



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:18 PM GMT

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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

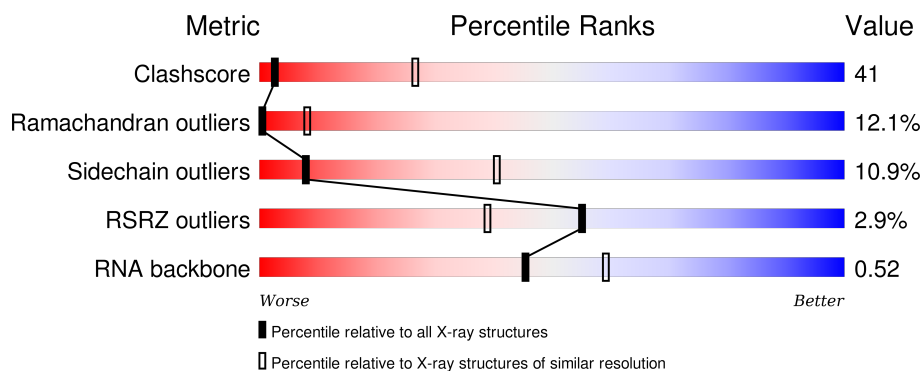
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

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.







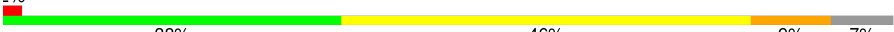
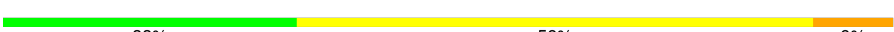
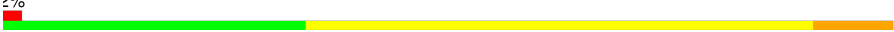





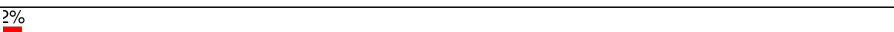

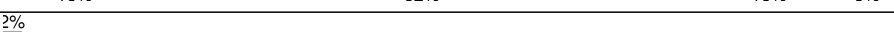

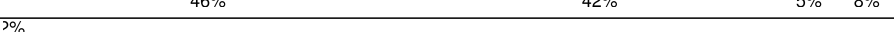

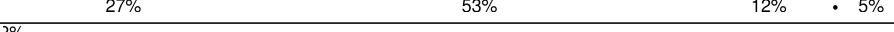
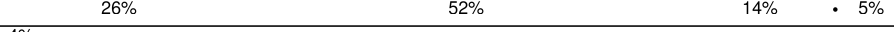
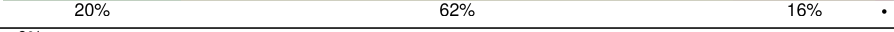
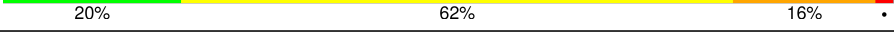


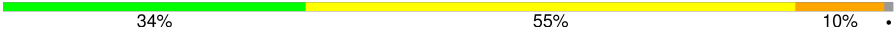
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>2%</div> <div>30% 56% 12%</div> <div>..</div> </div>
1	CA	1522	<div> <div>2%</div> <div>28% 58% 12%</div> <div>..</div> </div>
2	AB	256	<div> <div>25% 50% 15%</div> <div>8%</div> </div>
2	CB	256	<div> <div>23% 52% 15%</div> <div>8%</div> </div>
3	AC	239	<div> <div>22% 50% 14%</div> <div>13%</div> </div>


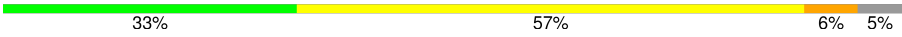


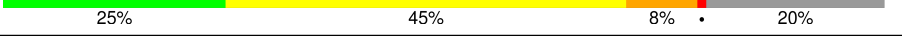
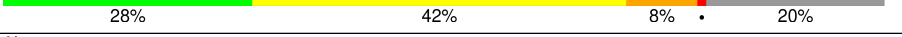
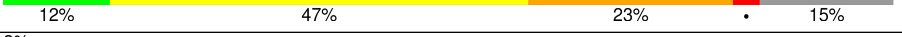

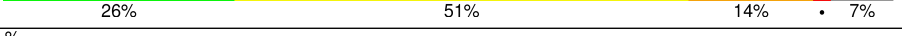
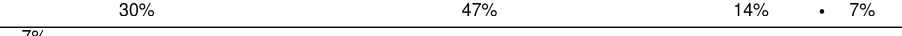
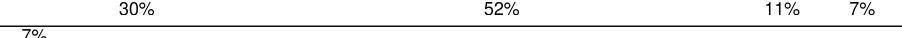
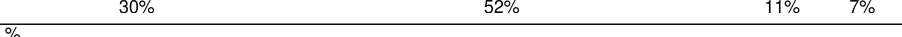

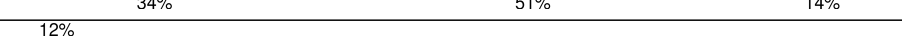


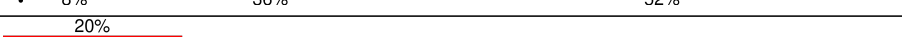

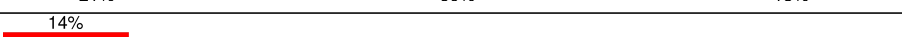




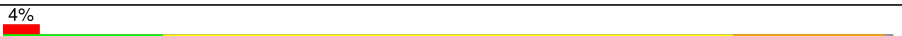

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Mol	Chain	Length	Quality of chain
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	

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Mol	Chain	Length	Quality of chain
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	

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Mol	Chain	Length	Quality of chain
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	
40	DE	206	

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Mol	Chain	Length	Quality of chain
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	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	
52	DU	118	
53	BV	101	

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Mol	Chain	Length	Quality of chain
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	FUA	AY	701	-	-	-	X
59	FUA	CY	701	-	-	X	X
60	GDP	AY	702	-	-	X	-
60	GDP	CY	702	-	-	X	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

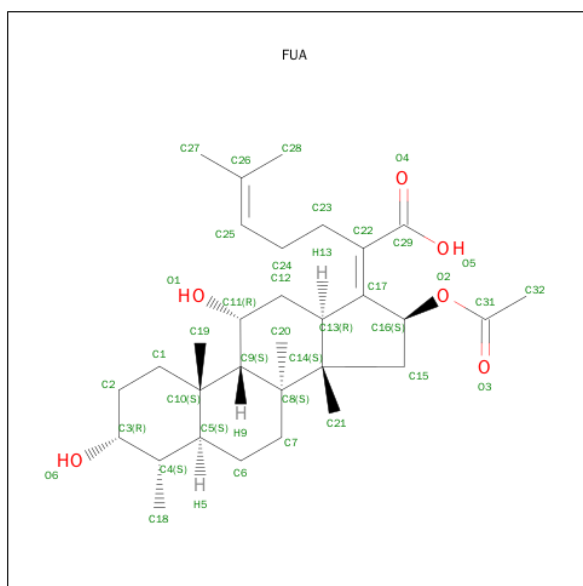
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B4	1	Total	Zn	0	0
			1	1		

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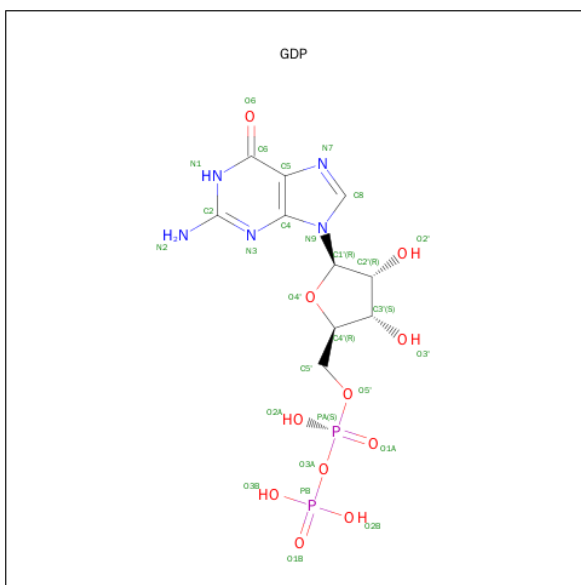
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	CN	1	Total	Zn	0	0
			1	1		
58	AN	1	Total	Zn	0	0
			1	1		
58	B9	1	Total	Zn	0	0
			1	1		
58	D9	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1	1		
58	CD	1	Total	Zn	0	0
			1	1		
58	AD	1	Total	Zn	0	0
			1	1		

- 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:  $C_{10}H_{15}N_5O_{11}P_2$ ).



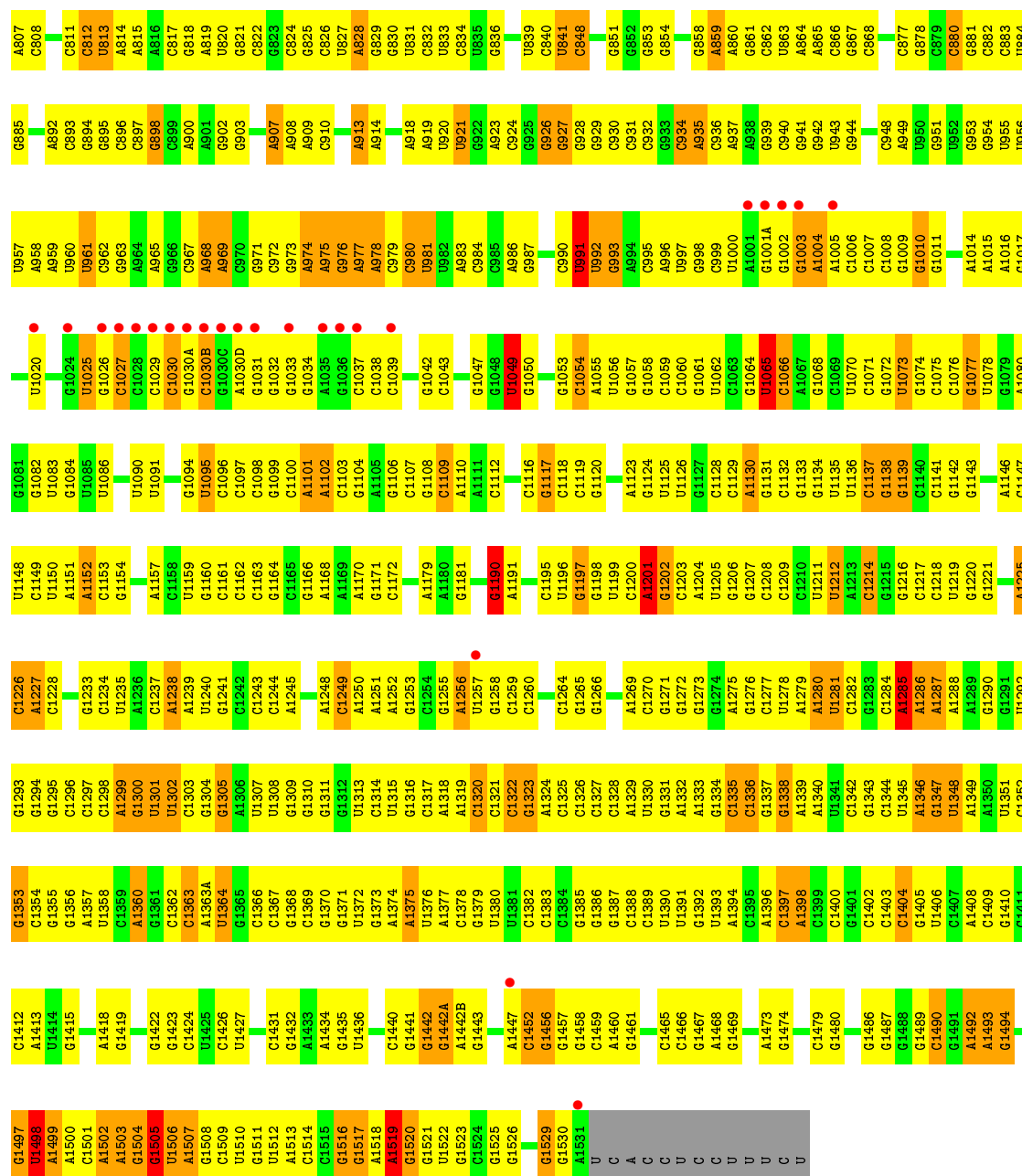
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
60	AY	1	Total 28	C 10	N 5	O 11	P 2	0	0
60	CY	1	Total 28	C 10	N 5	O 11	P 2	0	0

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

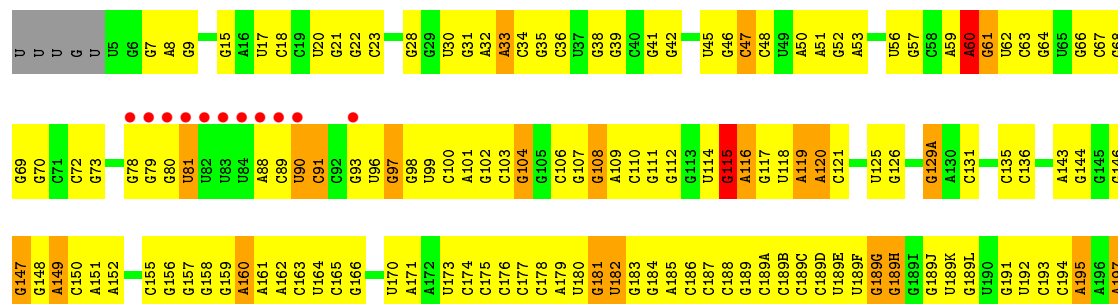
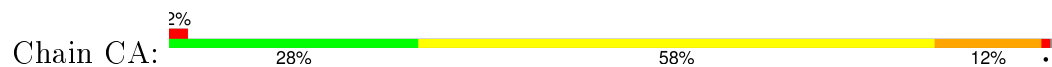
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	1	Total Mg 1 1	0	0
61	CY	1	Total Mg 1 1	0	0







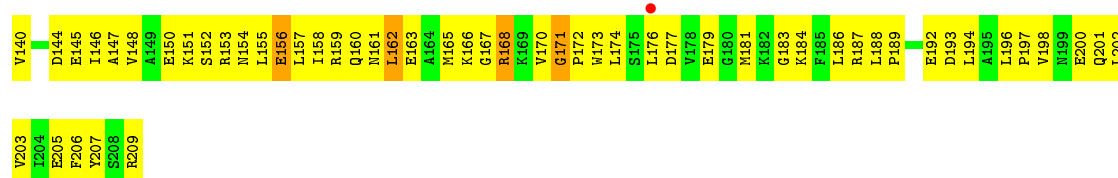
• Molecule 1: 16S RIBOSOMAL RNA



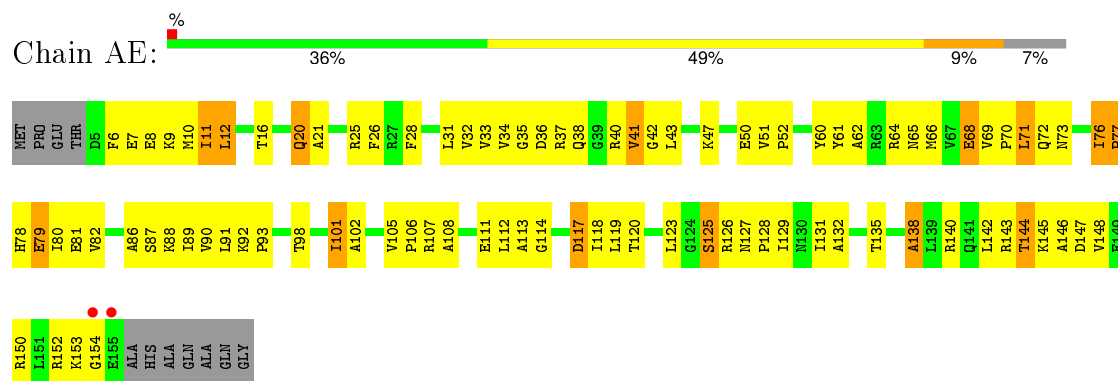
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G1283	C1214	C1137	C1071	C1006	G944	G867	A792	C719	U652	U571	U498	C418	U358	C289	C201
C1284	G1215	G1138	G1072	C1007	G945	C868	A793	G720	A653	A572	A499	C419	U359	C290	U202
A1285	G1216	G1139	U1073	C1008	A946	C877	A794	G721	G656	A573	G501	G422	A360	C291	U203
A1286	C1217	G1140	G1074	G1009	G947	C878	G797	U722	A574	A574	G502	G423	A361	G292	U204
A1287	C1218	G1141	G1075	G1010	G948	C879	G798	U723	G657	G575	G503	G424	G362	G293	G216
A1288	U1219	G1142	C1076	G1011	A949	C880	A802	G724	G658	G576	G504	G425	A363	U294	C217
A1289	G1221	U1143	G1077	A1014	U950	G881	A803	G725	G660	G577	G505	G426	A364	U296	C218
G1290	U1220	U1144	U1078	A1015	U951	G882	U804	G726	G661	G578	G506	U427	U365	G297	C219
A1291	A1146	A1147	G1079	A1016	U952	C883	G804	U727	G662	G579	A509	U428	C366	G298	G220
A1292	C1226	U1148	G1081	A1017	G954	C884	U807	G728	G663	G580	A510	U429	U367	G299	C221
A1293	A1227	U1149	U1082	G1017	U955	C885	C808	G731	G664	U582	U568	A430	U368	A300	U222
G1295	C1228	U1150	U1083	U1020	U956	G886	G808	G736	G665	A583	G511	A431	C369	G301	U223
C1296	U1221	A1151	G1084	U1021	U957	A892	C811	U737	G666	G584	G512	U434	C370	G302	C224
C1297	C1233	A1152	U1085	U1025	U958	C893	C812	A738	G667	G585	U513	C435	C371	C308	C235
C1298	U1234	G1153	U1086	G1026	A959	C894	U813	C738	G671	C586	U514	C436	C372	G309	C236
A1299	U1235	G1154	U1087	G1027	U960	C895	U814	C739	U672	G587	G515	U437	A373	G310	C237
G1300	A1236	U1155	U1088	C1028	U961	C896	A814	U740	G673	G588	G516	U438	A374	C311	C238
U1301	C1237	A1157	U1091	C1029	G962	C897	A815	U741	G674	U591	G517	A439	U375	C312	C239
U1302	U1238	C1158	U1092	C1030	G963	C898	A816	G742	A675	G592	G518	U441	C376	C313	C240
C1303	A1239	U1159	G1094	G1030A	A964	C899	C817	U743	U676	G593	C519	U442	C377	C314	C241
G1304	U1240	G1160	U1095	G1030B	A965	A900	G818	C744	U677	G594	G520	C443	C378	C315	C242
A1305	G1241	C1161	C1096	G1030C	G966	A901	A819	C745	G680	U598	G521	C444	C379	A315	C243
G1306	C1242	C1162	C1097	A1030D	C967	G902	U820	C746	C681	C600	G522	C445	C380	G316	U244
C1243	C1244	C1163	C1098	G1031	A968	G903	G821	C747	C682	C601	G523	C446	C381	C317	C245
U1308	A1245	G1164	G1099	G1032	A969	A907	G822	C748	G683	A602	C524	U447	A382	C320	A246
G1309	C1246	C1165	C1100	G1033	U970	A908	G823	C749	G684	C603	C525	C448	C379	C321	G247
A1310	U1247	C1166	A1101	G1034	C972	A909	G824	U751	G685	G604	C526	C449	C384	C322	C248
G1311	A1248	A1168	G1102	A1035	G973	C910	G825	G752	U686	U608	C527	C451	C385	U323	U249
G1312	C1249	A1169	G1103	G1036	A974	C911	G826	G753	U687	A608	G528	C452	C386	C324	C250
A1250	A1251	U1170	G1104	C1037	A975	A913	U827	G754	A687	A609	G529	C453	U387	A325	G251
C1314	C1252	G1171	A1105	C1038	G976	A914	A828	G755	G688	G610	G530	C454	C388	C326	G254
G1315	G1253	C1172	C1107	C1039	A977	G914	G829	U756	C689	A389	A532	C455	A391	G327	G255
C1316	U1254	U1173	C1108	G1042	C979	A918	U831	U757	U692	U534	A533	C456	G392	A328	U256
A1318	G1255	U1174	G1109	C1043	U980	A919	C832	C758	G693	A535	A535	C457	A393	C330	G257
A1319	A1256	G1181	A1110	G1044	U981	U920	U833	C759	A694	C536	G537	C458	A394	G331	G260
C1320	U1257	G1190	C1111	G1047	U982	U921	C834	G765	A695	G538	A538	C459	C395	G332	U261
C1321	G1258	A1191	C1112	G1048	C983	G922	U835	A766	A696	G539	A539	C460	C396	G333	A262
C1322	C1259	U1192	G1113	U1049	C984	A923	G836	A767	G697	U626	G540	C461	A397	C334	A263
G1323	U1260	C1193	C1114	G1050	C985	C924	U837	A768	C698	G628	G541	C462	A398	C335	U264
A1324	C1261	G1195	G1115	G1051	A956	G925	U839	C769	C699	G629	G542	C463	C399	C336	G265
C1325	G1264	U1196	C1116	G1052	C986	G926	U840	C770	G700	G630	C543	C464	C400	C337	G266
C1326	U1265	G1197	C1117	C1053	U927	G927	U841	C771	A702	A632	G544	C465	C401	A338	G267
C1327	G1266	U1198	G1118	A1055	G928	G928	C848	U772	G703	G633	C545	C466	C402	G342	C268
U1328	U1267	U1199	C1119	U1056	U992	G929	G851	U773	A704	G634	G546	C467	C403	U343	C269
A1269	C1270	C1200	G1120	G1057	G993	C930	G852	G774	G708	G635	A547	C468	C404	A344	A270
A1330	G1271	G1201	G1121	G1058	A994	C931	G853	G775	C709	G636	U552	C469	G405	C345	C271
G1331	C1272	G1202	U1125	C1059	C995	C932	G854	G776	G710	G637	C554	C470	U404	G346	G275
A1332	U1273	C1203	U1126	C1060	A996	G933	G854	G777	G711	G638	C555	C471	U405	A347	G276
A1333	G1274	A1204	G1127	G1061	U997	C934	G854	A778	C708	G639	C556	C472	G406	A348	G277
C1334	U1275	U1205	C1128	U1062	G998	C935	A858	G779	G709	G640	C557	U486	A408	G349	G278
C1335	A1276	G1206	G1129	C1063	C999	C936	A860	A780	G712	G641	C558	C487	A412	G350	G284
C1336	G1277	G1207	U1130	G1064	U998	C937	G861	A781	A713	C559	C557	C488	A413	G351	G285
G1337	C1278	C1208	G1131	U1065	A1001	U938	G862	A782	G714	U646	C560	C489	G414	C352	G286
G1338	U1279	C1209	C1132	C1066	G1001A	G939	C863	G783	G715	C647	U560	C490	A415	A353	G287
A1339	A1280	G1210	G1133	A1067	G1002	C940	U864	G784	A716	G648	U561	G491	A416	G354	G288
A1340	U1281	C1211	U1134	U1068	G1003	G941	A865	G785	C717	G650		G492	G416		
U1341		U1212	U1135	C1069	A1004	G942									



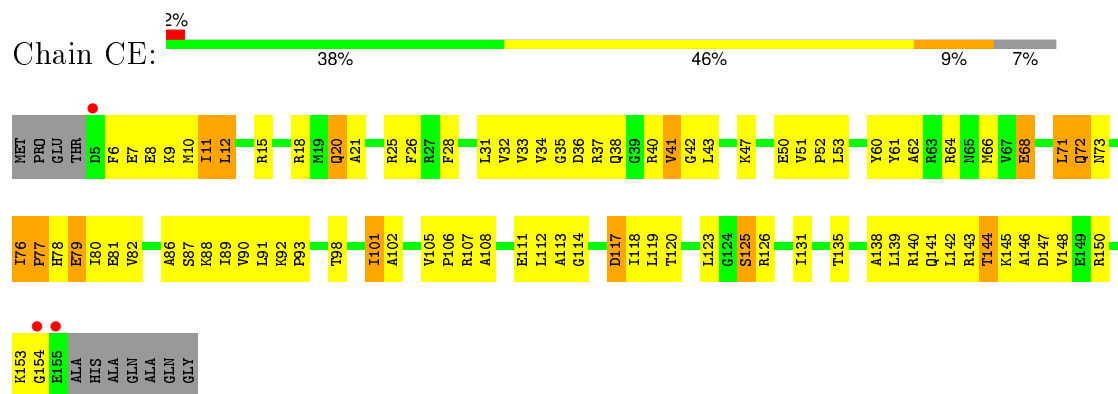




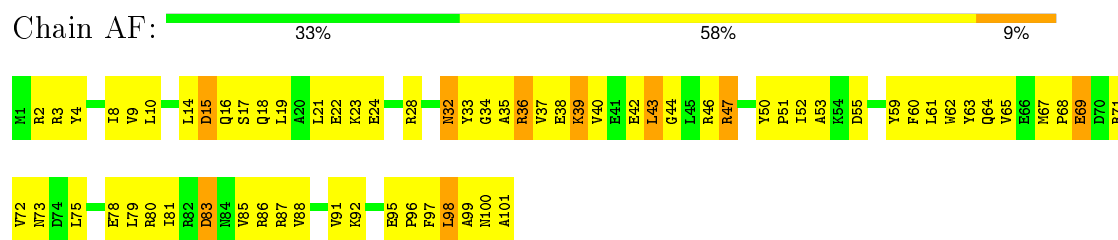
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



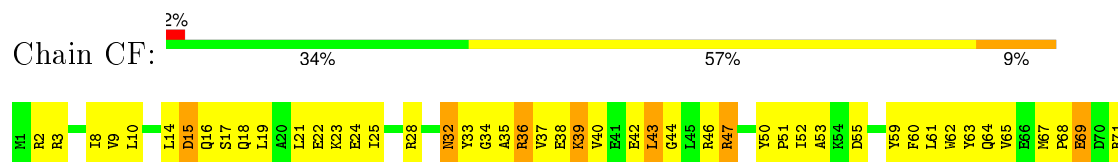
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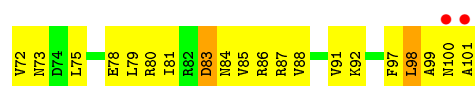


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

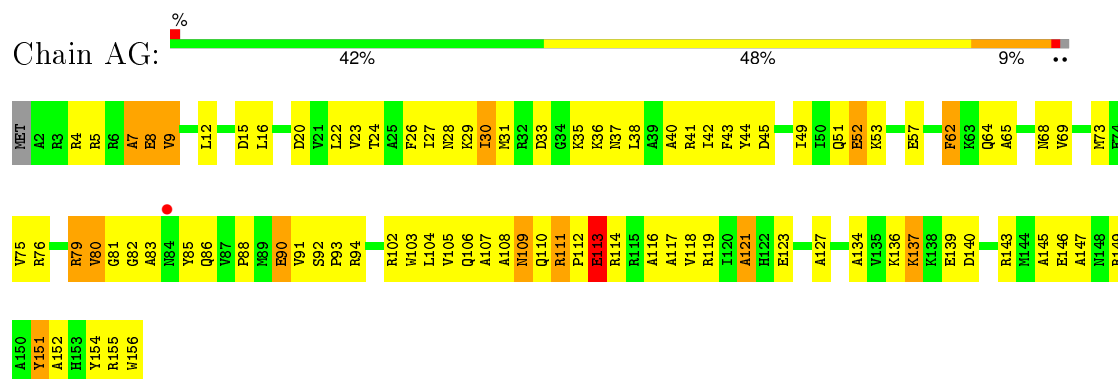


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

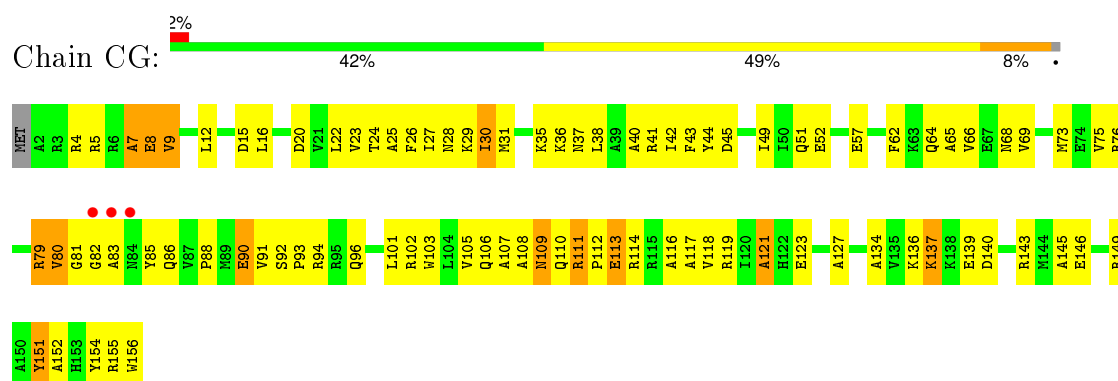




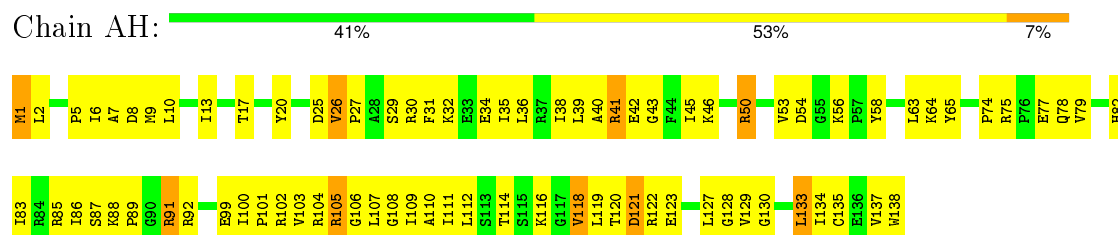
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



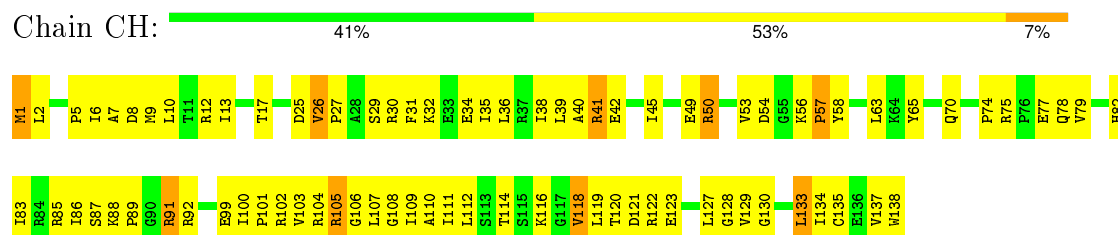
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



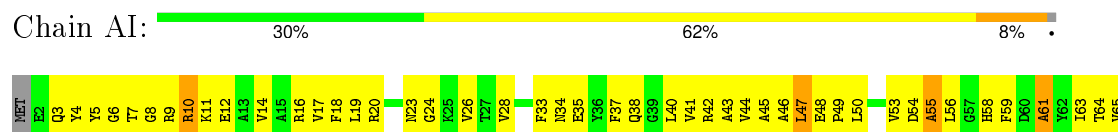
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



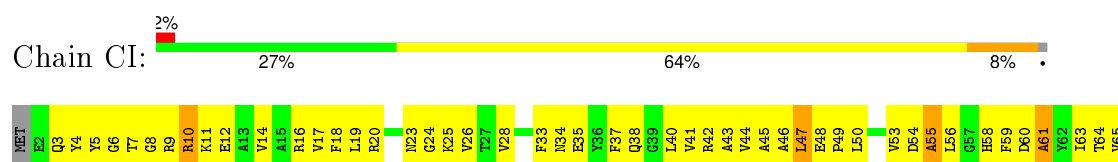
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



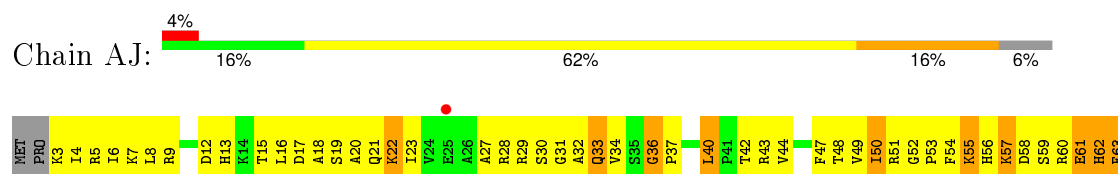
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



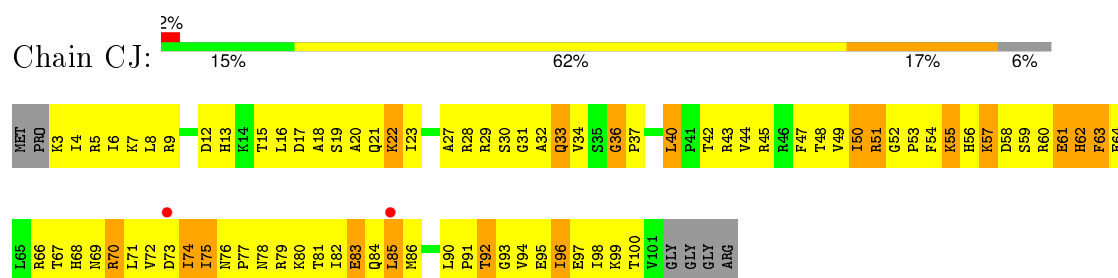
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



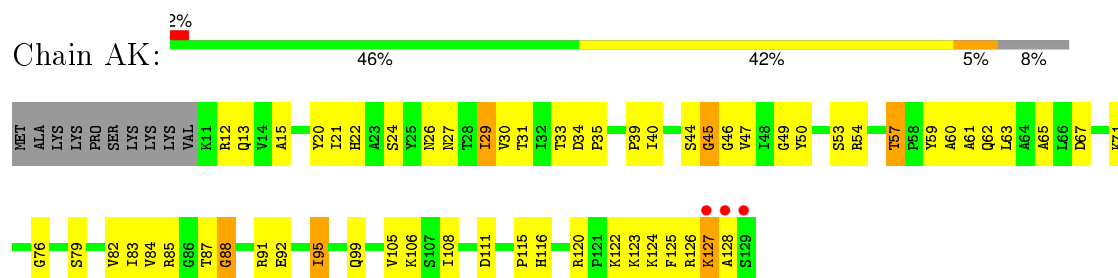
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

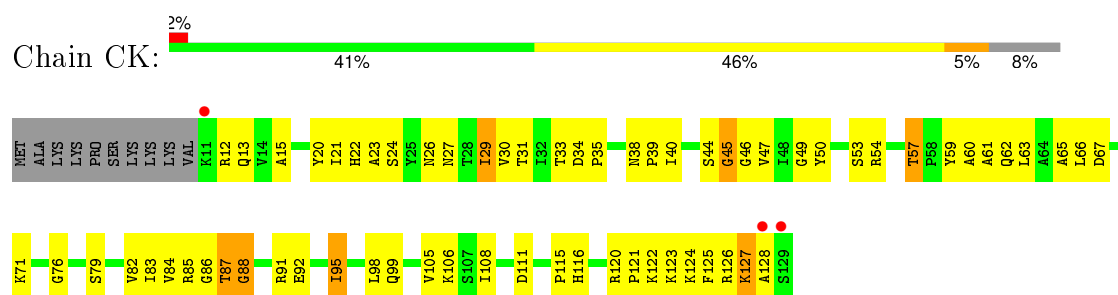


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

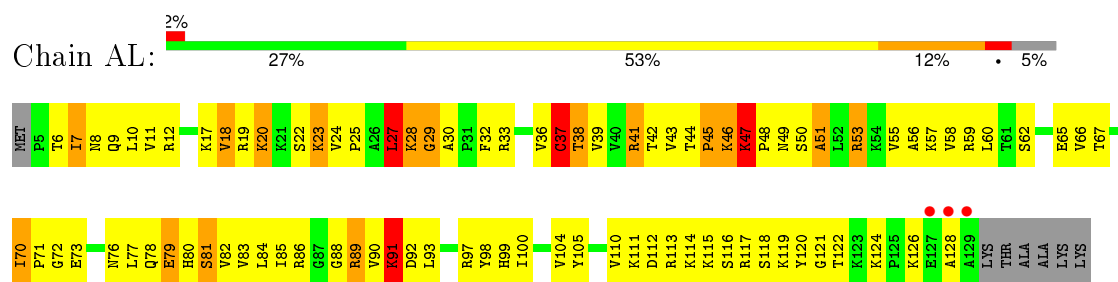


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

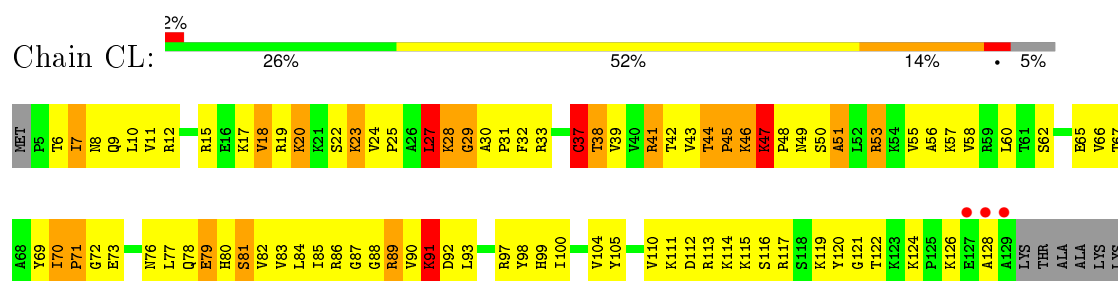




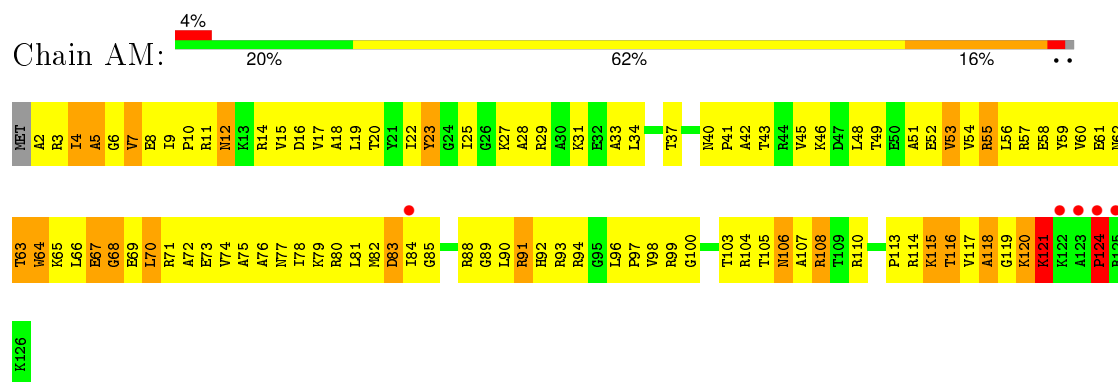
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



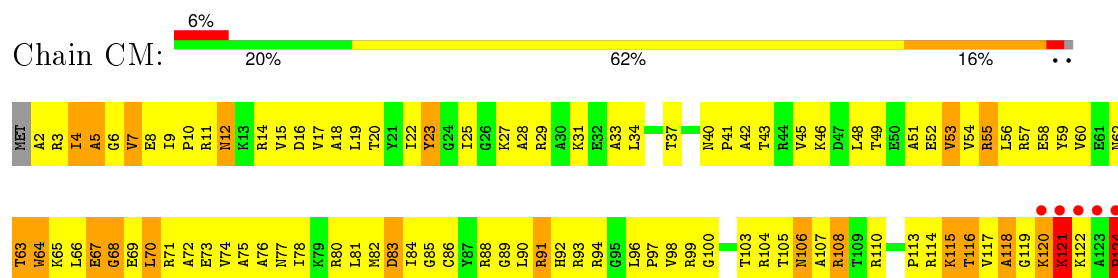
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



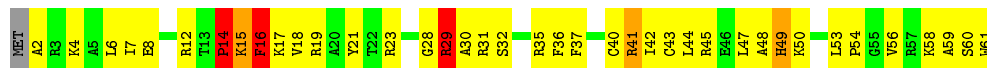
• Molecule 13: 30S RIBOSOMAL PROTEIN S13





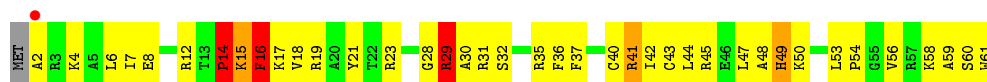
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 34% 54% 5% 5% .



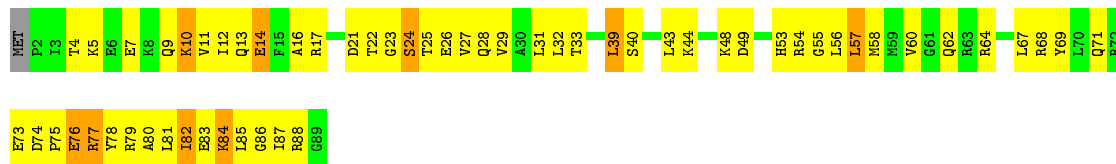
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN: 2% 34% 54% 5% 5% .



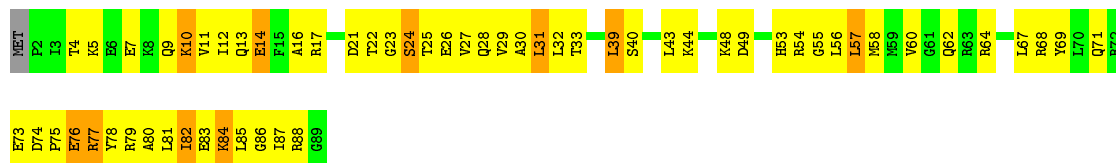
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 34% 55% 10% .



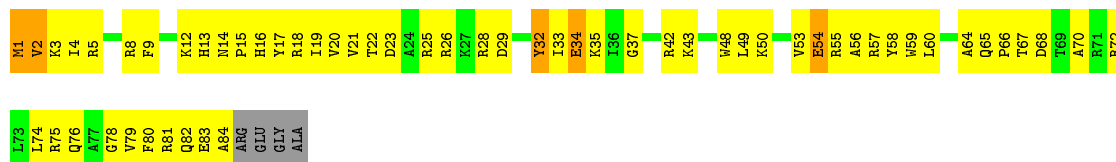
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO: 33% 55% 11% .



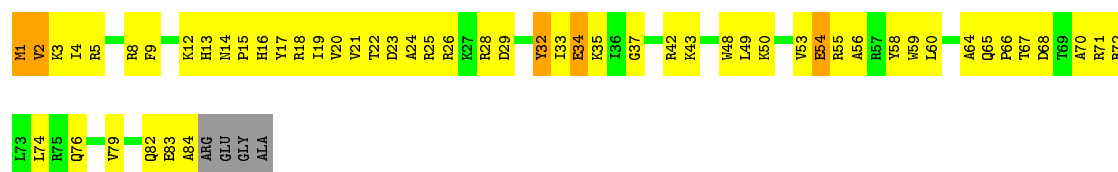
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 30% 60% 6% 5%

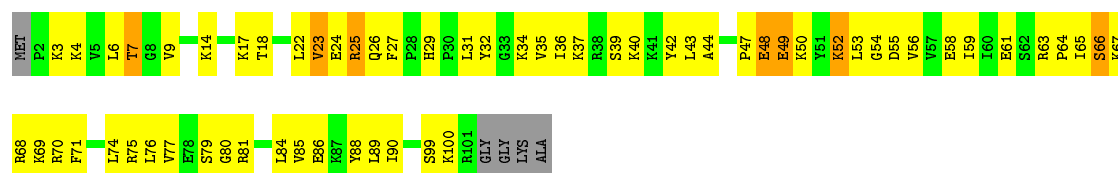


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

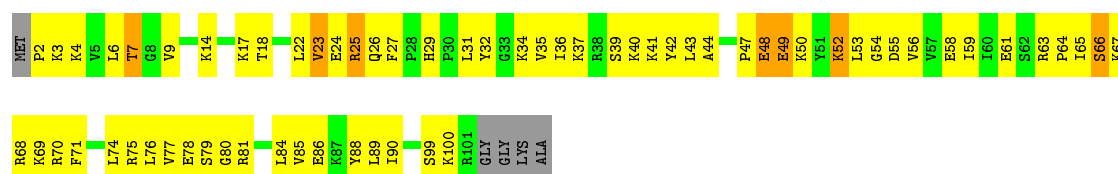
Chain CP: 33% 57% 6% 5%



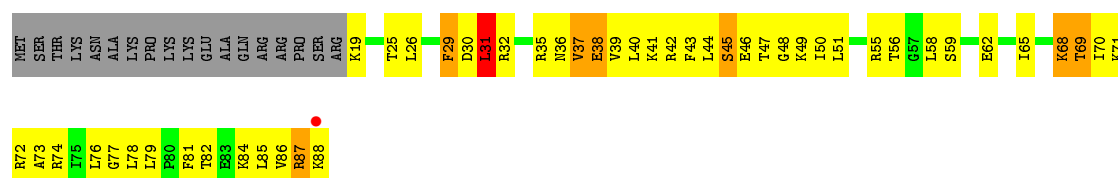
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



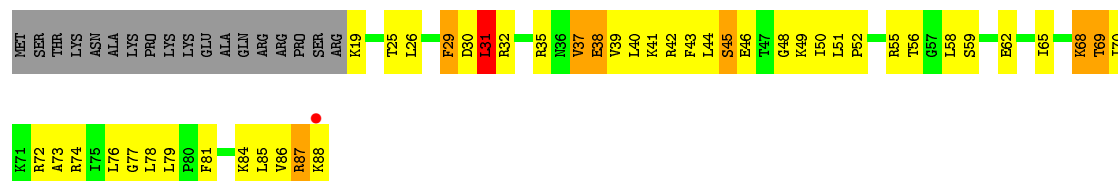
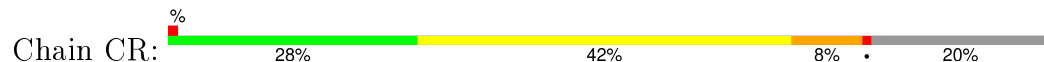
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



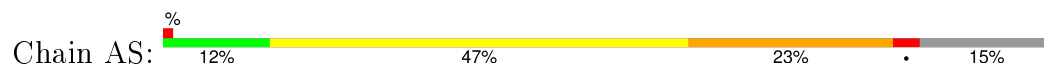
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 18: 30S RIBOSOMAL PROTEIN S18



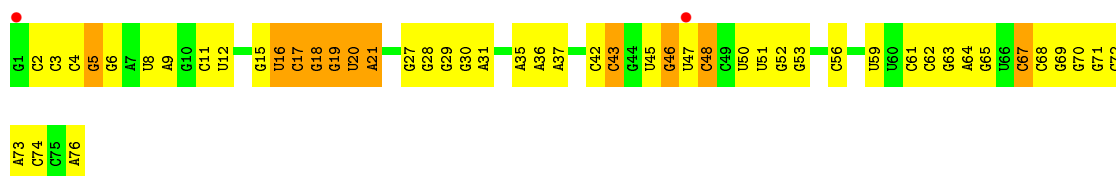
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



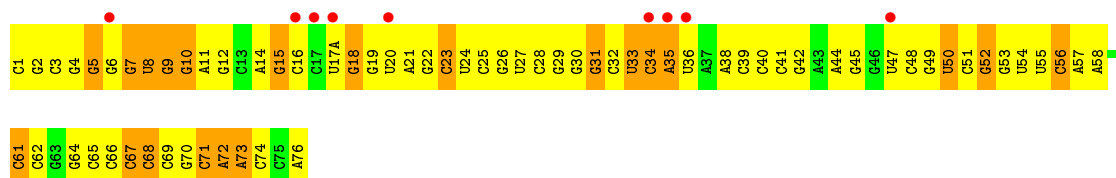
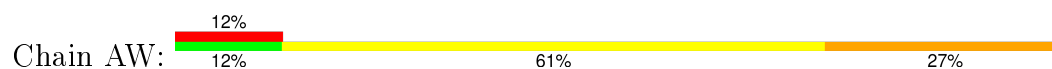




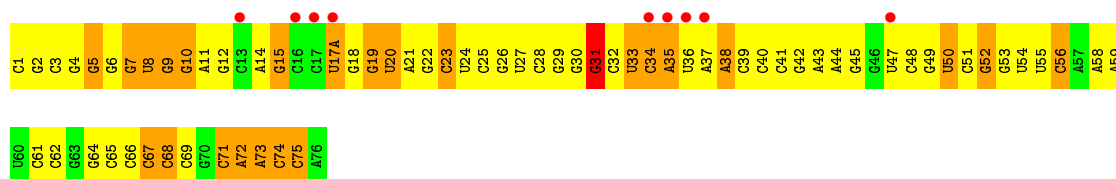
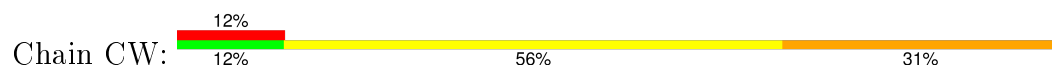
- Molecule 22: MRNA



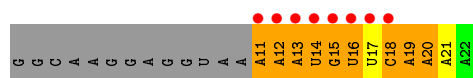
- Molecule 23: RNA



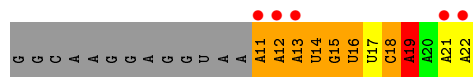
- Molecule 23: RNA



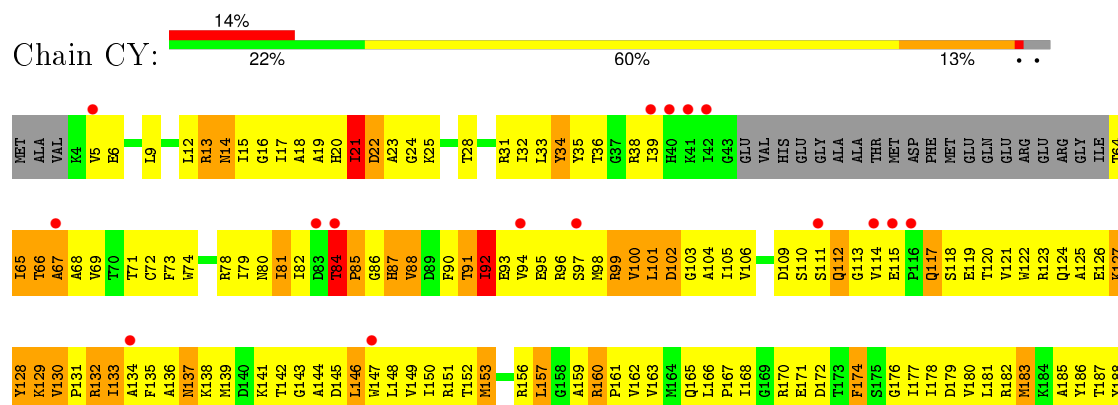
- Molecule 24: RNA

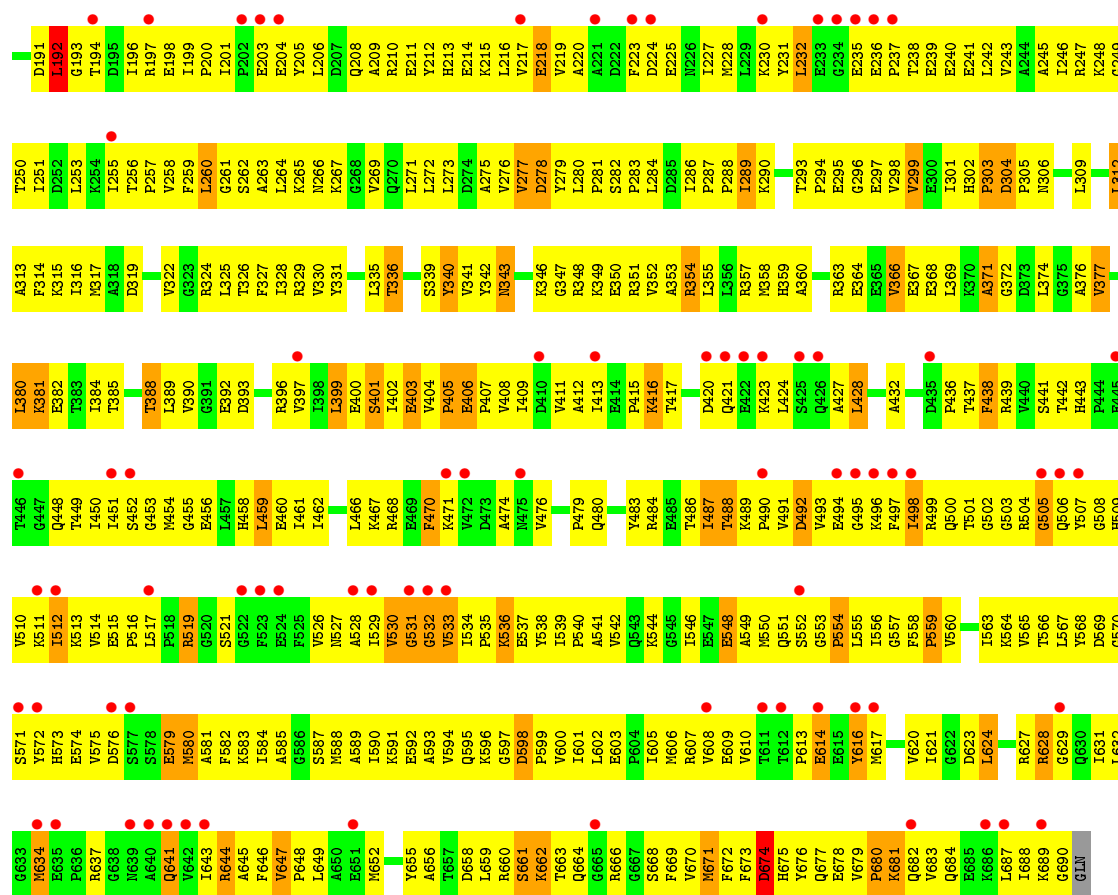


- Molecule 24: RNA



- Molecule 25: ELONGATION FACTOR G





● Molecule 26: 50S RIBOSOMAL PROTEIN L27

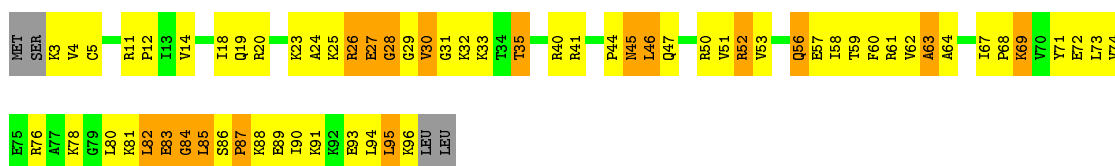


● Molecule 26: 50S RIBOSOMAL PROTEIN L27

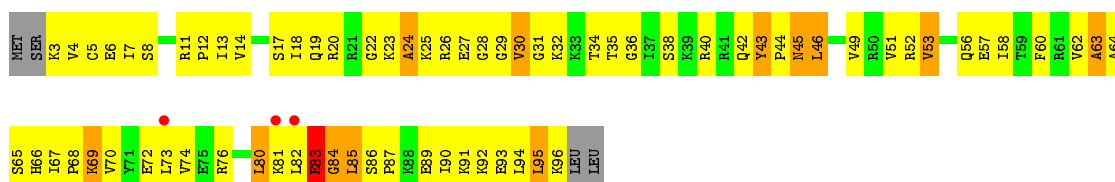


● Molecule 27: 50S RIBOSOMAL PROTEIN L28

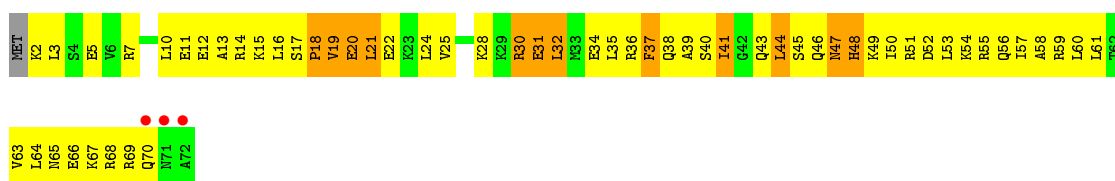




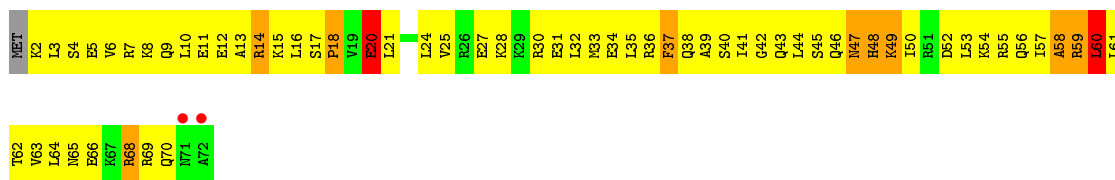
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 28: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L29



• Molecule 29: 50S RIBOSOMAL PROTEIN L30

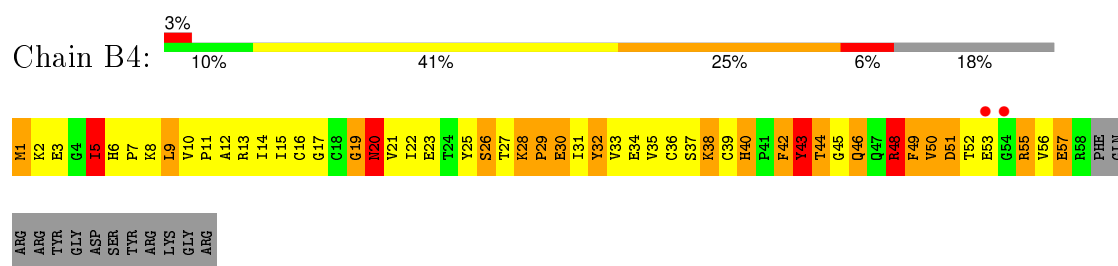


• Molecule 29: 50S RIBOSOMAL PROTEIN L30

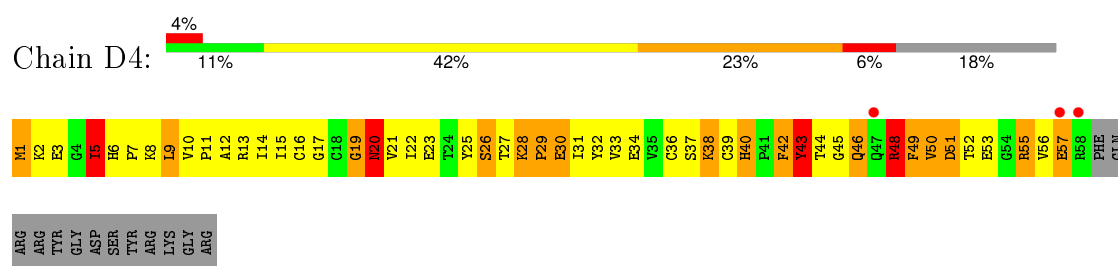


• Molecule 30: 50S RIBOSOMAL PROTEIN L31

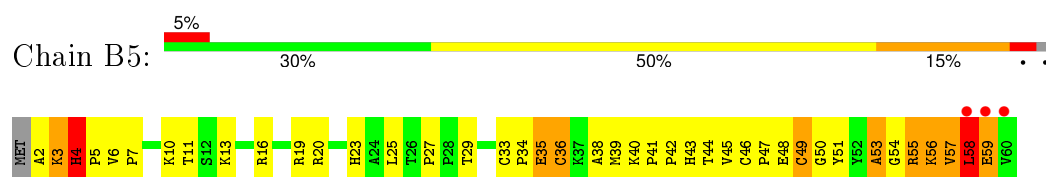




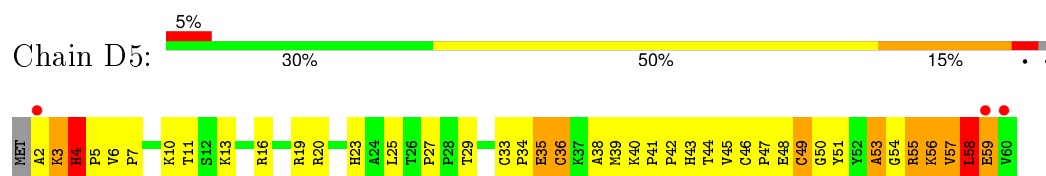
- Molecule 30: 50S RIBOSOMAL PROTEIN L31



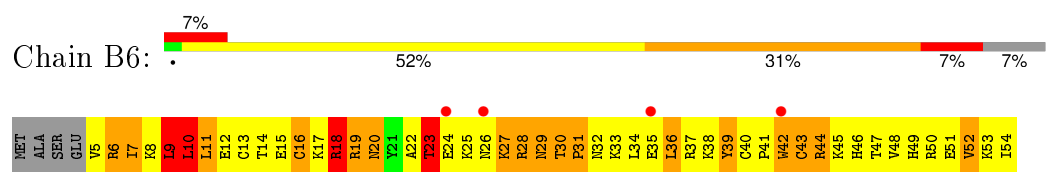
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



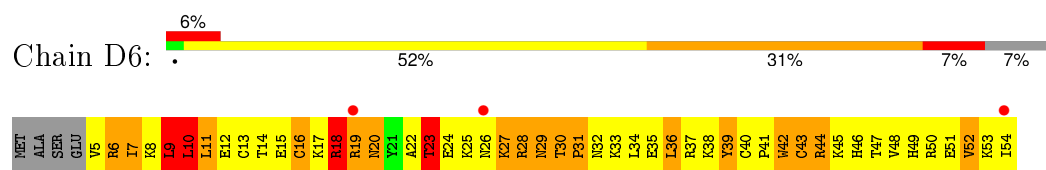
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



- Molecule 32: 50S RIBOSOMAL PROTEIN L33

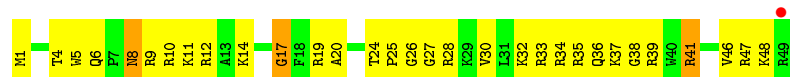


- Molecule 32: 50S RIBOSOMAL PROTEIN L33

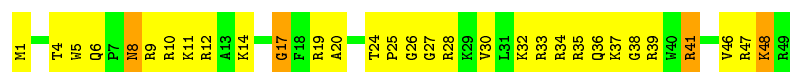


- Molecule 33: 50S RIBOSOMAL PROTEIN L34

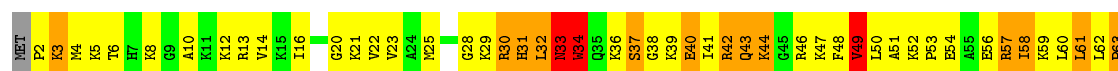




• Molecule 33: 50S RIBOSOMAL PROTEIN L34



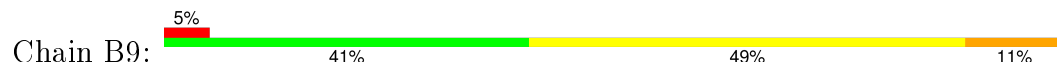
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



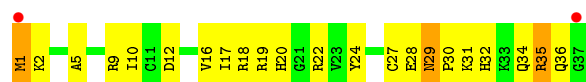
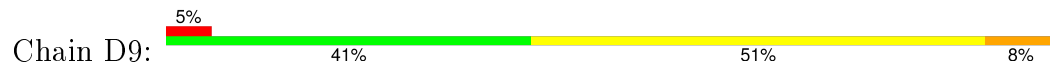
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 36: 23S RIBOSOMAL RNA



U969	A901	U833	G770	G704	G654B	G598	A526	U459	G307	U271E	A207	G68
C970	C902	C834	A773	A705	G654E	G611	C527	A460	A310	C271F	C208	C69
C971	C903	A835	A774	A706	G654F	G601	A528	A461	A311	G271G	C209	G70
C972	C904	G836	A775	G707	G654G	G602	A529	G462	G383	G271H	C210	A71
A973	U905	C837	G776	C708	G654H	A603	G530	G463	U384	G271I	G211	U72
G974	G906	G838	G777	U709	G654I	A604	C531	U464	C385	G271J	G212	A73
G975	U907	C839	A777	G710	A654J	G605	A532	G465	G386	U271K	A213	A74
G975A		C840	G778	G711	G654K	U606	G533	G467	G387	U271L	G214	G139A
G976	A910	A841	U779	G712	G654L	U607	U534	G468	C318	U271M	A140	G75
G977	G977	G780	G781	G713	G654M	A608	C541	G469	C319	U271N	A141	C76
G978	U913	C844	A782	A718	G654N	A609	G544	A472	G321	U271O	A142	C77
G979	C914	G845	A783	C719	G654O	G610	C545	G473	A322	G271P	G143	A78
A980	C915	C846	A784		C611	C612	A547	A474	G323	G271Q	A144	G62
A981	G916	U847	G785	A722	G654P	G613	A548	U475	A324	C271R	G145	G83
A982	A917	G848	G786	G723	G654Q	G614	A549	U476	G325	C271S	G146	A84
A983	A918	A849	U787	G724	G654R	U614	G549	G478	G326	G271T	A149	G85
A984	U922	C850	A788	U725	G654S	U614A	G551	A479	G327	G271U	G226	C86
C985	C923	G851	A789	G726	A654T	G614B	G552	A480	A228	U271V	A227	C87
C986	C924	G852	G790	A727	G614C	G615	G553	A481	A229	C271W	A228	G88
G987	C925	G853	C791	G728	A614D	G616	U554	G482	U230	U272A	A229	U90
A988	C926	C857	G792	G729	G656	G617	U555	A483	C154A	U272B	U155	A92
A989	A926	U858	G793	C730	U657	G618	G556	A484	U156	G272C	U157	G93
A990	G927	G859	G794	G731	G659	G619	G557	G485	U158	G272D	U158	G94
C991	G928	A860	C795	G732	G660	A621	U558	C486	G152		G152	G94A
C992	G929	G861	C796	G733	G661	G622	G559	G487	G153		G153	G95
G993	G932	G862	G797		G662	G623	C560	G488	G154		G154	G96
A996	A934	G863	G798	C737	G663	G624	G561	G489	G155		G155	G97
G997	G935	G864	G799	G738	G664	G625	U562	G490	U156		U156	G98
C998	C936	G865	A800	G739	G665	U626	G563	A492	G174		G174	G99
	U937	G866	G801	U740	G666	A627	C564	G493	G175		G175	G100
	G938	U868	A802	G741	G667	G628	C565	G494	G176		G176	G101
G939	A940	G869	U803	G742	G668	G629	U566	G495	G177		G177	G102
G940	G941	A870	G804	G743		G630	A567	U500	G178		G178	A103
C1005	A941	G871	G805	G744	C671	A631	U568	G501	G179		G179	G106
C1006	G942	G872	C806	G745	G673	G634	U569	A502	G180		G180	C107
A1009	U943	C876	U807	A746	G674	C635	A571	G503	G184		G184	U108
A1010	G944	U877	G808	U747	A675	C636	A572	U504	U185		U185	G109
G1011	A945	G878	G809	G748	A676	A637	G573	A505	G186		G186	G110
U1012	G946	G879	U810	C749	A677	G638	C574	G506	G187		G187	A111
C1013	G947	G880	U811	A750	G680	U639	A575	A507	G188		G188	U112
G1014	G948	G881	C812	A751	G681	C640	U576	G508	G189		G189	G113
U1015	G949	G882	U813	A752	G682	C641	G577	C509	A190		A190	U114
G1016	C950	G883	C814	C753	G683	G642		C510	A191		A191	C115
G1017	A953	C884	C815	C754	G684	A643	C581	U511	C192		C192	C116
C1018	G954	C885	C816	C755	G685	A644	G582	G512	G117		G117	G118
C955	C955	A887	C817	C756	A686	C645	A572	A505	G193		G193	A119
A1020	G956	C888	G818	U757	G687	A646	C584	A514	A195		A195	U120
A1021	G957	C889		C758	U688	G647	G585	A515	A196		A196	G121
G1022	U958	A890	A821	G759	A689	G648	A586	C516	A197		A197	G122
U1023	G959	G892	G823	G760	G689	G649	C587	C517	A198		A198	G123
G1024	A960	C893	A824	U762	G690	C650	U588	G518	G261		G261	U200
G1025	C961	C894	C825	G763	U694	G651	C589	U519	C262		C262	G124
U1026	G962	U895	U826	A764	G695	C652	A590	U448	A263		A263	G125
A1027	U963	A896	U827	G765	G696	A653	C591	A449	C264		C264	U202
A1028	C964	C897	U828	C766	G697	A654	G592	G522	U269		U269	A126
G1029	G965	A898	A829	U767	G698	G654A	G593	C523	C203		C203	A127
A1030	G966	G830	G830	G768	G699	G654B	U594	U524	A204		A204	G128
				G769	U703	G654C	C595	U525	G205		G205	C129
									U206		U206	G130

G2029	U1798	G1878	U1798	G1714	A1634	G1559	U1489	G1422	U1352	G1285	A1220	A1156	A1095	U1033
A2030	G1799	C1882	G1799	G1717	G1635	G1565	A1490	G1423	A1353	A1286	C1221	G1157	A1096	G1034
A2031	C1800	G1883	C1800	G1718	A1636	C1566	G1491	G1424	A1354	A1287	C1221A	G1158	A1097	U1035
A2032	G1801	G1883	G1801	G1719	A1637	A1566	G1492		G1355	U1288	C1222	U1159	A1098	G1036
U2033	A1802	A1884	A1802	G1720	G1638	G1567	G1493	A1428	G1358	G1290	G1223	G1160	G1099	G1037
U2034	A1803	A1885	A1803	G1721	G1639	G1568	A1494	G1429	A1359	C1291	G1224	G1161	C1100	G1038
G2035	G1804	C1886	G1804	A1722	C1640	A1569	A1495	C1430	A1360	C1292		G1162	U1101	G1039
G2036	U1805	C1887	U1805	A1723	C1644	G1573	A1496	C1431	A1361	C1293		G1163	C1102	C1040
G2037		G1888		G1740		G1574	A1497	U1431	G1362	U1294	G1227	G1164	A1103	G1041
G2038	A1809	A1889	A1809	A1741		C1574		U1432	A1362	C1295	G1228	U1165	C1104	G1042
G2039	G1810		G1810		G1647	C1575	U1503	C1432	C1363	C1296		U1166	U1105	C1043
C2040	G1811		G1811	G1744	G1648	U1576	C1504	A1434	G1364	G1297	G1231	C1167	G1106	G1044
U2041	A1812	A1900	A1812	C1745	G1649	C1577	C1505	U1433	G1365	C1298		U1168	G1107	A1045
A2042	G1813	A1901	G1813		G1650	U1578	C1506	G1435	A1365		G1232	G1169	U1108	A1046
G2043	G1814		G1814	G1747A	G1651	A1579		G1436	A1366	G1299	U1234	G1170	U1109	G1047
	A1815		A1815	G1748	A1652		C1509	U1437	A1367	U1300	G1235	G1171	C1110	A1048
G2046	G1816	G1653	G1816	A1749	A1654		A1509A	U1438	G1368	A1301	G1236	G1172	G1111	G1049
	G1817	A1654	A1817		A1654	A1583	A1509B	A1439	G1369	A1302	G1237	A1174	A1112	A1050
G2049	G1818	A1655	G1818	G1754	A1655	C1584	G1510	G1441	G1374		G1238	U1175	U1113	G1051
C2050	U1819	A1656	U1819	A1755	C1656	A1586	C1511	G1442	C1375	C1306	U1240	G1176	G1114	C1052
A2051	G1820	G1657	G1820	G1756	C1657	A1587	U1512		C1376	A1307	U1241	A1177	G1115	C1053
G2052	A1821	U1757	A1821	G1757	C1658	C1588	C1513	A1445	G1377	A1308	A1242	G1178	C1116	U1061
G2053	G1910	G1658	G1910	G1758	G1659	C1589	U1514	C1445A	A1378	G1309	G1243	C1179	G1117	G1054
G2054	G1822	G1659	G1822	G1759	C1660	U1590	G1515	G1446	A1379	G1310	G1244	C1180	G1118	G1055
G2055	G1823	A1912	G1823	A1759	G1661	G1591	G1516	G1447	G1380	G1311	G1245		G1119	G1056
G2056	G1824	G1662	G1824	A1760	G1662	C1592	G1517	G1448	G1381	U1312	A1246		G1120	A1057
A2057	A1825	C1663	A1825	G1761	C1663	G1593		G1449	G1382	U1313	G1247	G1183	G1121	G1058
	G1826	G1664	G1826	A1762	G1664	G1594	G1518	G1450	C1383	C1314	A1248	G1184	C1122	U1059
A2060	C1827	G1665	C1827	G1763	G1665	G1595	G1520	G1451	A1384	C1315	U1249	G1186	U1060	U1060
G2061	G1828	A1667	G1828	G1764	C1667	A1596	G1523	G1452	G1385	U1316	G1250	G1187	C1123	U1061
A2062	A1829	A1668	A1829		A1668	A1597	G1524	A1453	C1386	A1317	C1251	U1188	G1125	G1062
		A1669		G1767	A1669	C1598	G1525	U1455	C1387	C1318	G1252	A1189	A1126	G1063
G2065	C1836	C1670	C1836	U1768	C1670	C1599	G1526	G1455	G1388		G1253	G1190	A1127	U1065
	G1921	G1671	G1921	G1769	G1671	G1600	G1527		G1389	A1322	A1254	G1191	A1128	U1066
U2068	G1838	C1672	G1838	G1770	C1672	A1601	G1528	G1459	U1390	U1325	U1255	G1192	A1067	U1067
G2069	G1839	A1674	G1839	C1771	A1674	G1601	A1528A	G1461	U1391	G1326	G1257	G1193	A1132	G1068
G2070	U1841	A1675	U1841	G1772	A1675	G1605		C1462	A1395	C1327	C1258		U1133	A1070
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C2007	G1930	A1679	G1930	G1776	U1679	A1608	G1533	G1465	A1406	C1330	C1261	U1198	G1137	A1073
C2008	U1931	G1680	U1931	U1777	G1681	A1609	U1534	G1466	G1407	A1331		U1200	G1138	G1074
U2075	G1845	G1681	G1845	U1778	G1682	A1610	A1535		G1401	G1332	U1263		G1139	G1075
U2076	A1932	G1682	A1932	U1779	G1683	C1611	G1536	C1467	C1402	U1264	U1264	G1203	C1140	C1076
	G1933	C1683	G1933	A1780	C1683		G1537		C1403	C1333	G1265	A1204	U1141	A1077
U2011	A1847	G1684	A1847	G1781	C1684	A1614	G1538	A1472	G1403	U1334	A1265	A1205	U1142	
G2012	G1848	G1685	G1848	C1782	G1685	C1615	G1539	G1473	C1404	U1335	G1266	G1206	A1142A	C1080
A2013	G1850	A1686	G1850	C1783	A1686	A1616	G1540	C1474	U1405	A1336	U1267	C1207	A1143	U1081
C2014	U1851	A1690	U1851	A1783	A1689	G1617	G1541	G1475	U1406	G1337	A1268	G1208	G1144	U1082
A2015	C1852	A1691	C1852	A1784	A1690	A1618	A1542	C1476	G1407	G1338	A1269	G1209	C1145	U1083
U2016	G1853	G1692	G1853	A1785	G1692	G1619	C1543	A1477	C1408	G1339	C1270	A1210	C1146	
U2017	G1856	G1693	G1856	A1786	G1694		A1544	G1478	C1409	U1340	G1271	U1211	C1147	A1086
G2018	G1857	A1695	G1857	A1787	G1695	A1614	G1545	G1479	G1410	U1341	U1272	U1212	C1148	A1087
A2019	C1858	G1696	C1858	C1788	G1696	C1615	A1546	U1481	C1411		U1273	G1213	G1149	A1088
U2091	A1859	A1698	A1859	A1789	A1698	A1616	G1546	G1480	G1411	G1344	A1274	A1213	C1150	G1089
U2092	G1860	G1699	G1860	C1790	A1699	C1625		U1482	G1412	G1345	A1275	G1215	G1151	U1090
G2093	G1862	A1791	G1862	A1791	G1699		A1553	G1484	U1415	G1346	A1276	G1216	C1152	G1091
	U1943	G1948	U1943		G1948	U1629	A1554	G1485	G1416	G1347	G1277	G1217	C1153	G1092
A2019	U1944	G1949	U1944		G1949	G1630	A1555	G1486	G1417	A1348	A1278	G1218	G1154	U1094
U2098	G1950	C1866	U2098	U1794	C1710		G1556	G1487	C1417	A1349	G1279		A1155	
G2099	U1951	A1952	G2099	C1795	C1711	A1632	G1557		U1420			G1219		
U2099	A1876		U2099	U1796	C1712		C1557	G1488	G1421					
G2100	A1877		G2100	C1797	U1713	G1633	A1558							



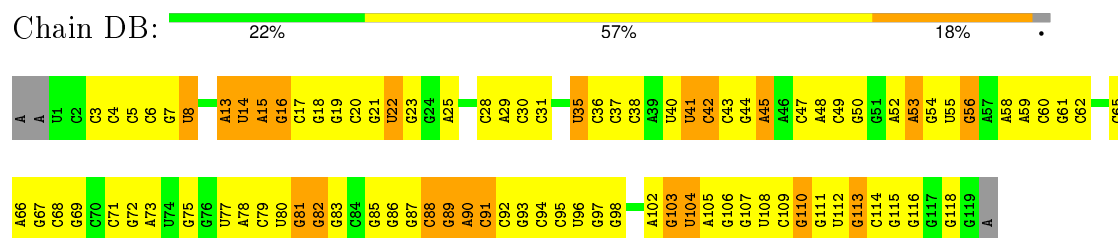




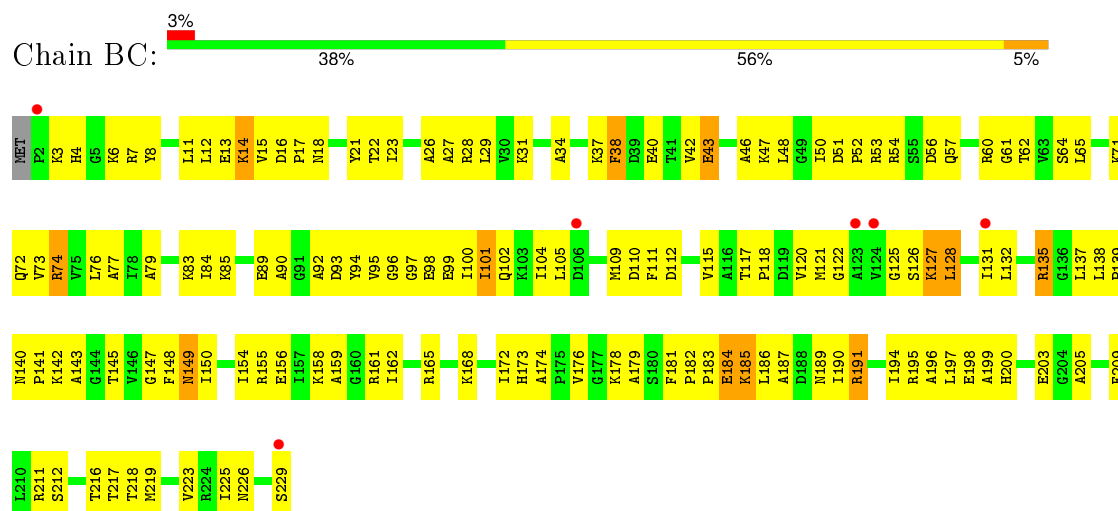




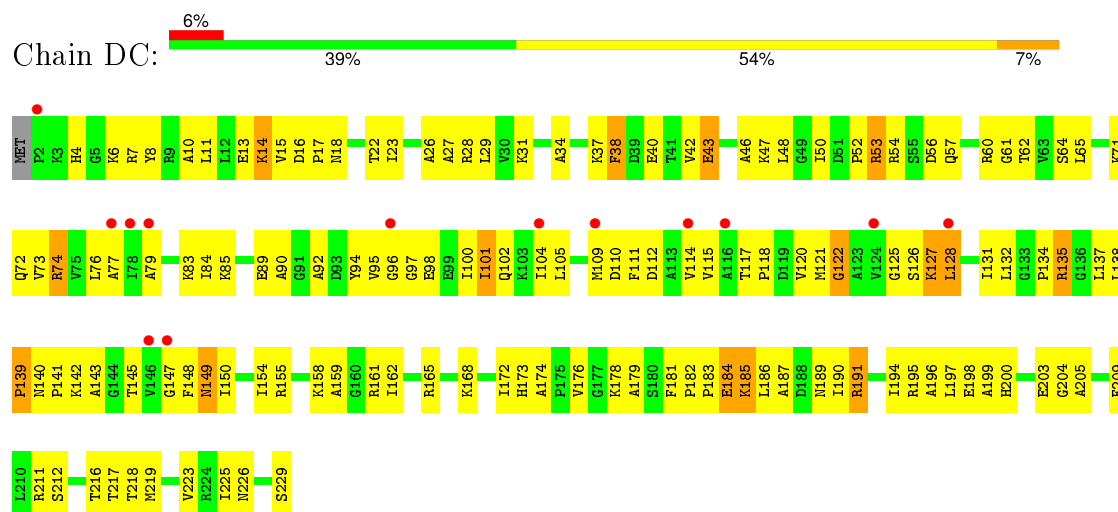
- Molecule 37: 5S RIBOSOMAL RNA



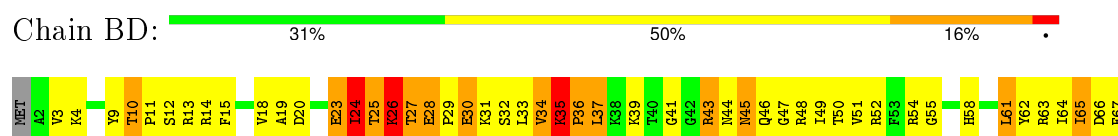
- Molecule 38: 50S RIBOSOMAL PROTEIN L1

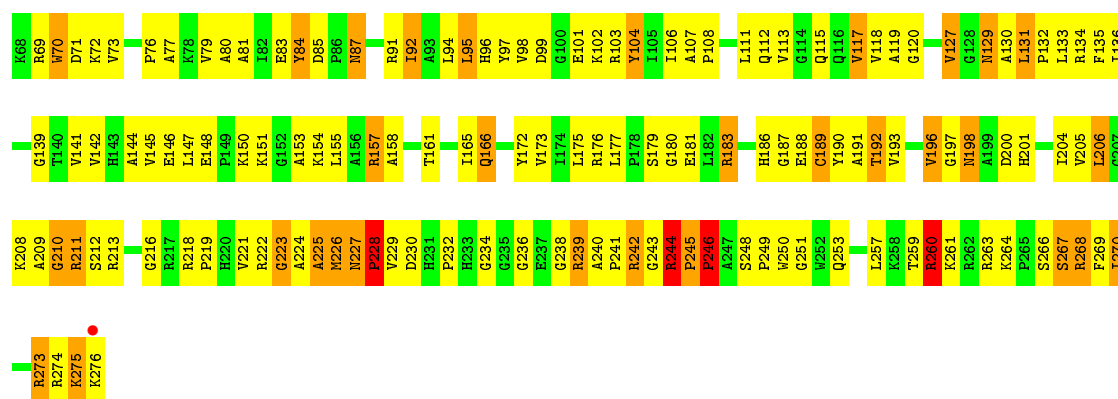


- Molecule 38: 50S RIBOSOMAL PROTEIN L1



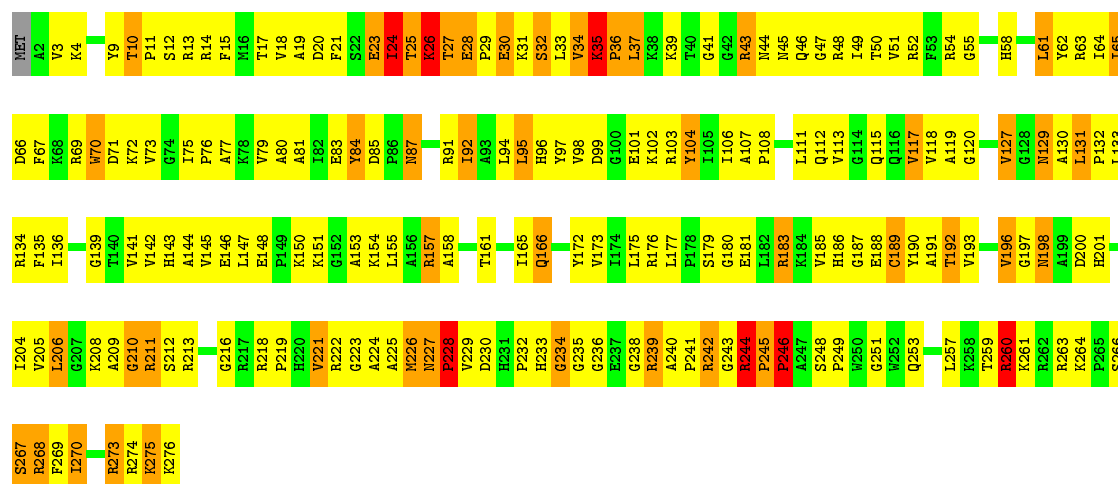
- Molecule 39: 50S RIBOSOMAL PROTEIN L2





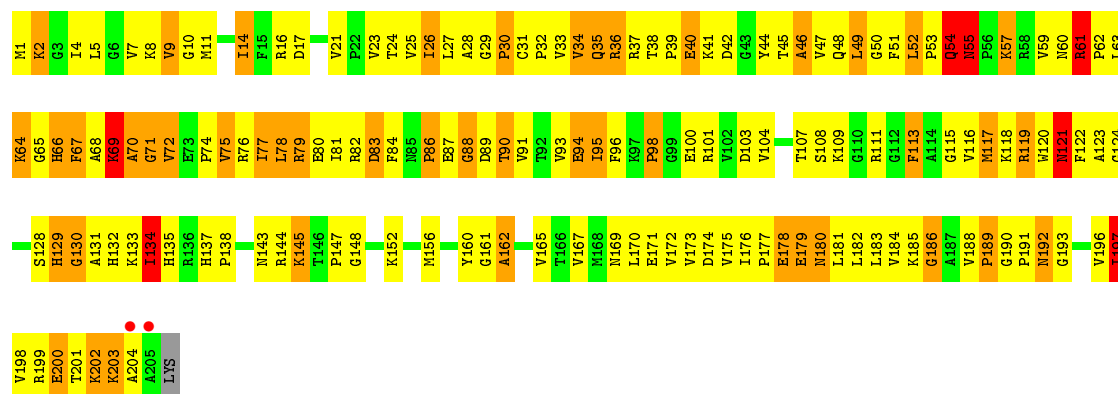
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD: 29% 52% 16%



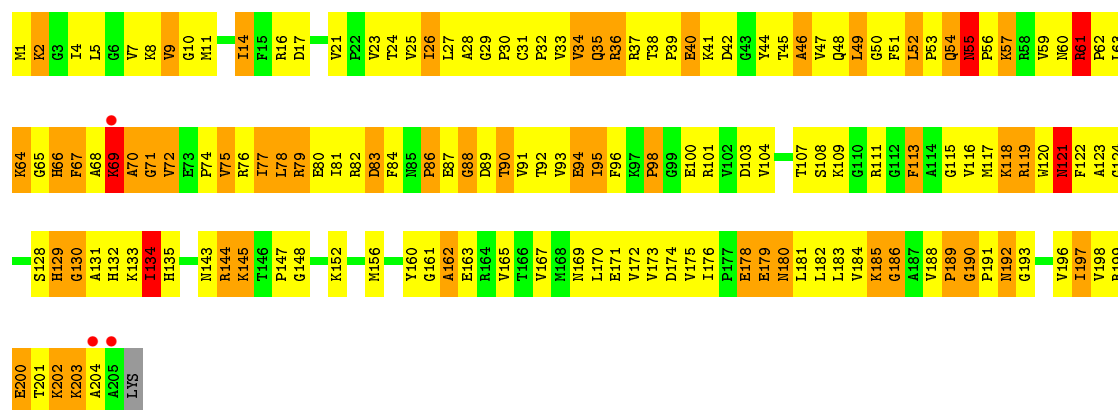
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain BE: 24% 50% 22%

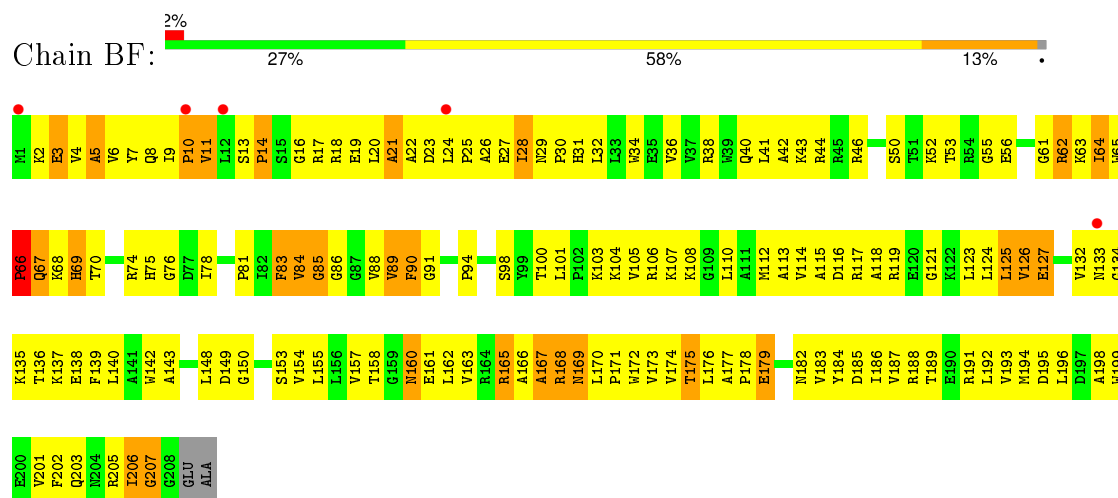


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

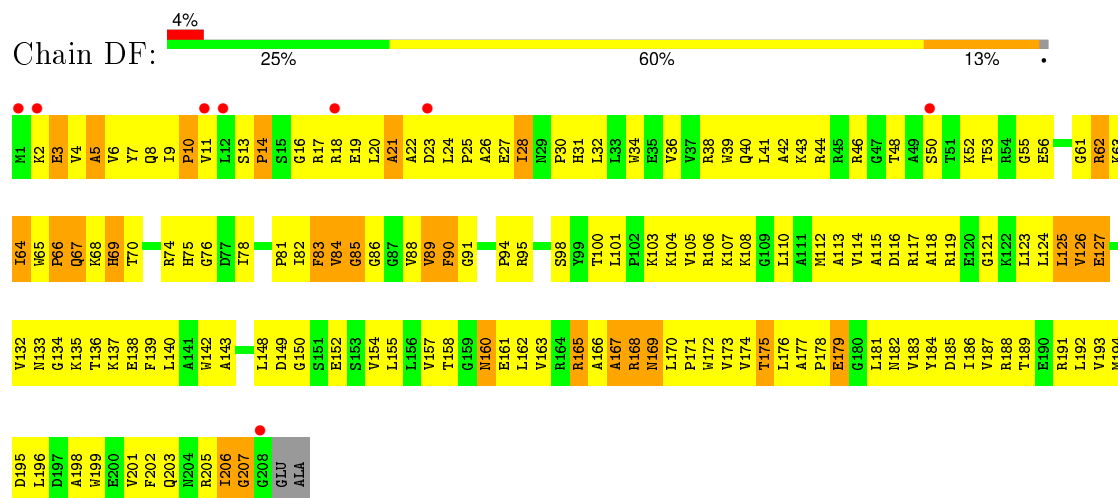
Chain DE: 24% 49% 24%



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

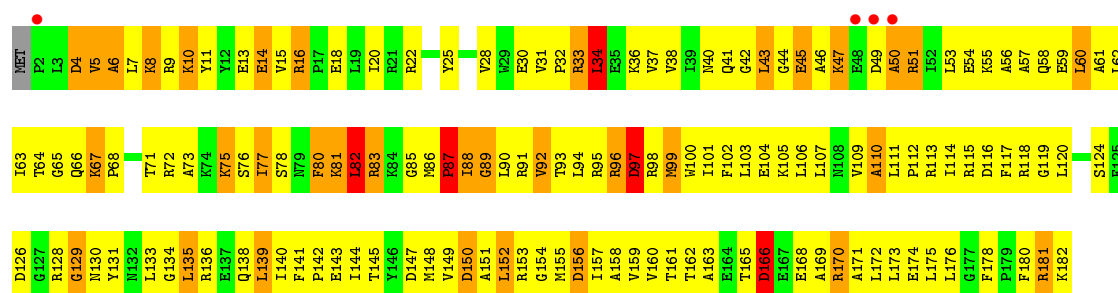


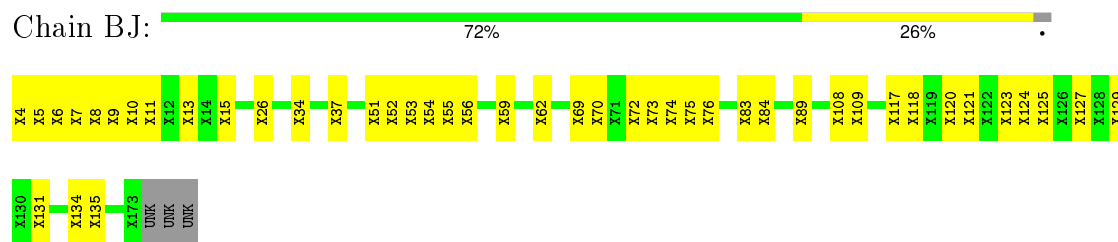
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



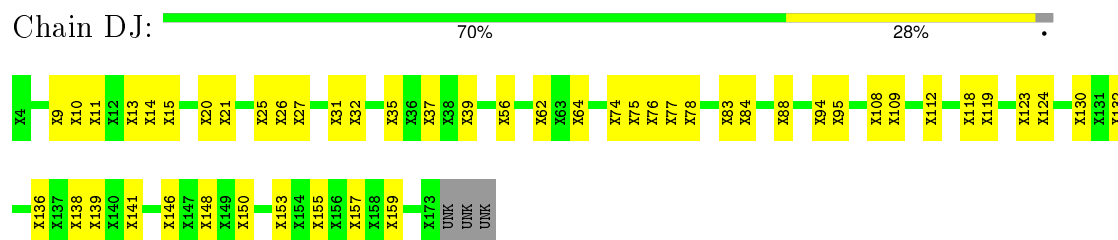
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



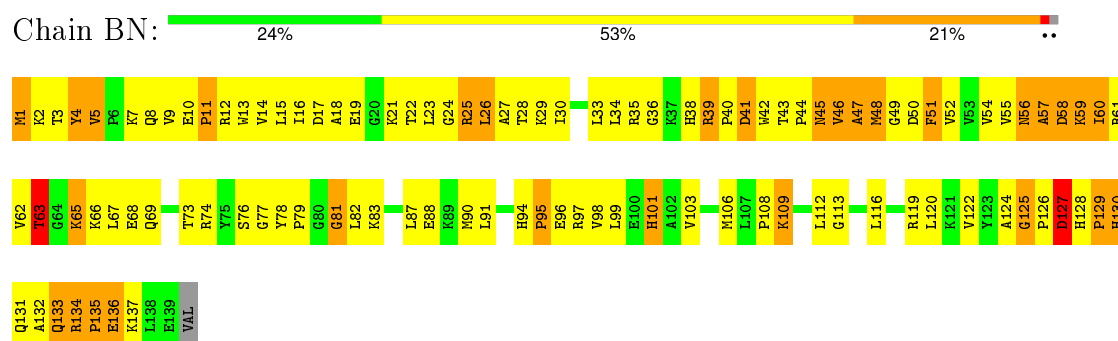




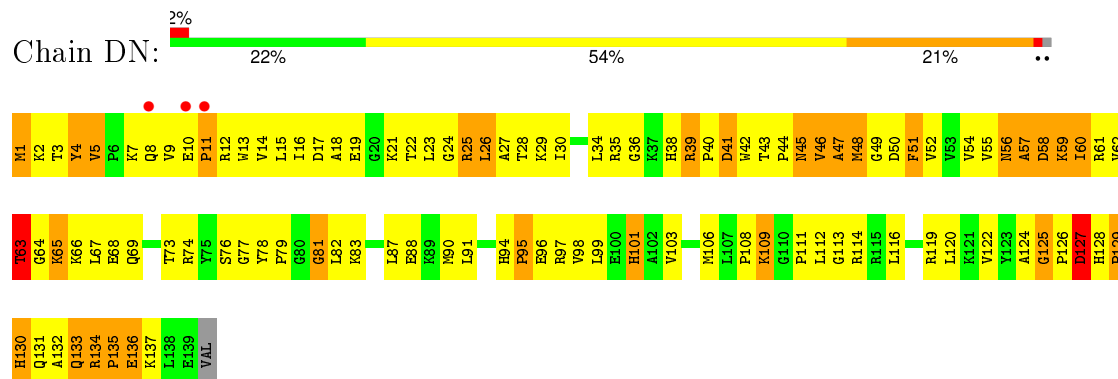
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



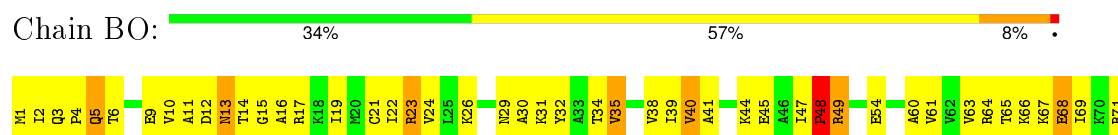
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

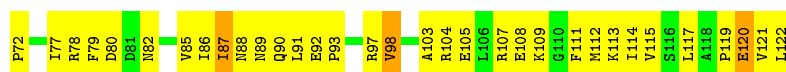


• Molecule 45: 50S RIBOSOMAL PROTEIN L13

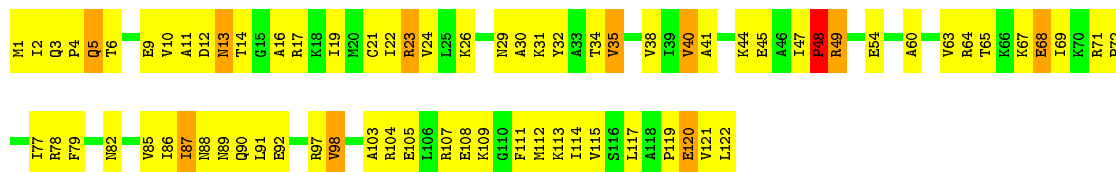


• Molecule 46: 50S RIBOSOMAL PROTEIN L14

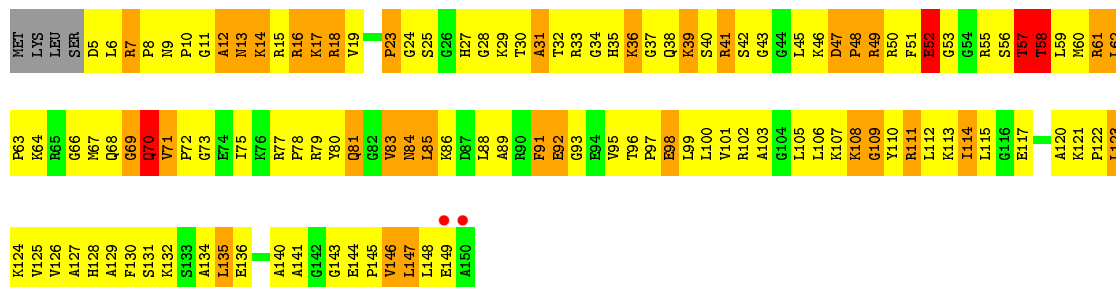
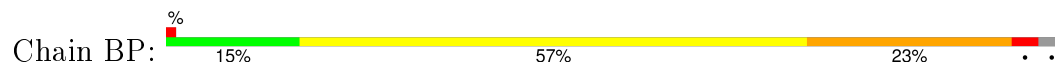




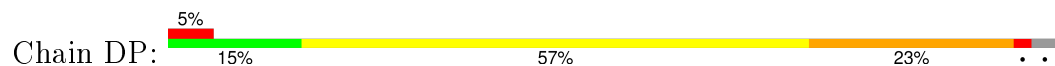
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



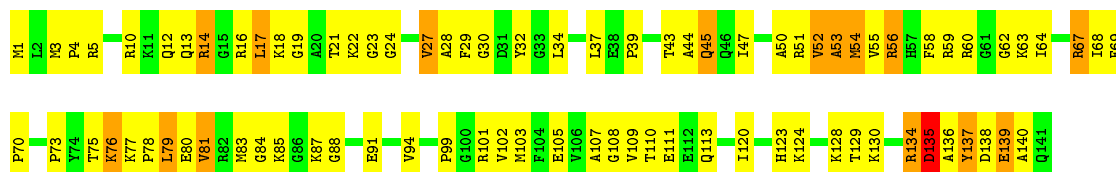
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



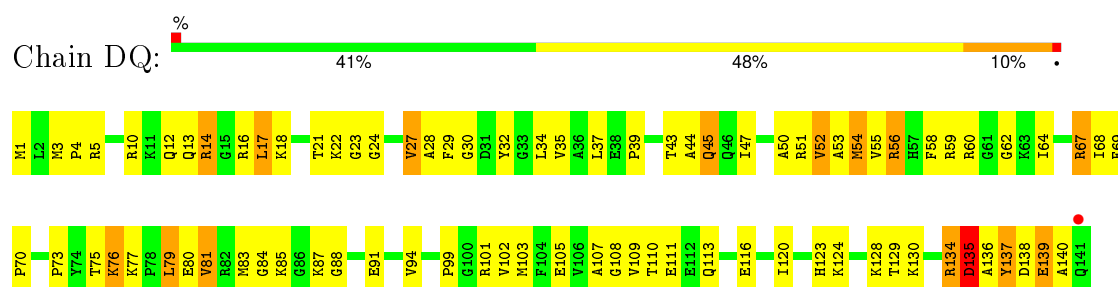
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



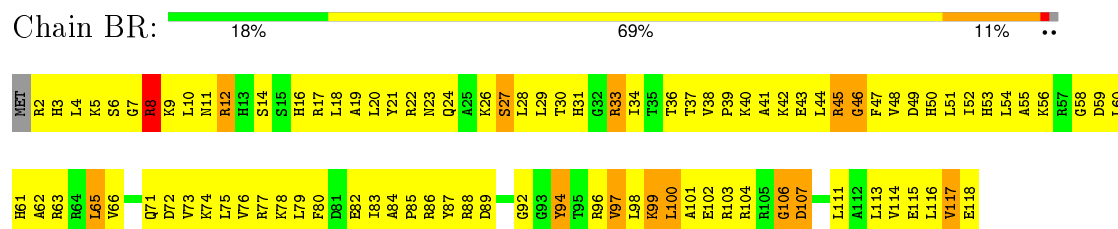
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



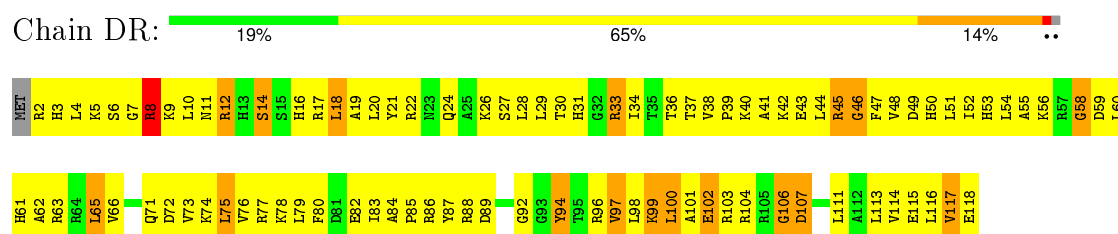
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



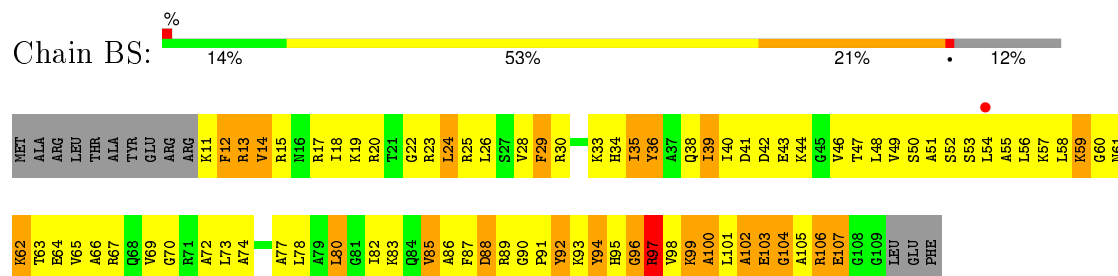
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



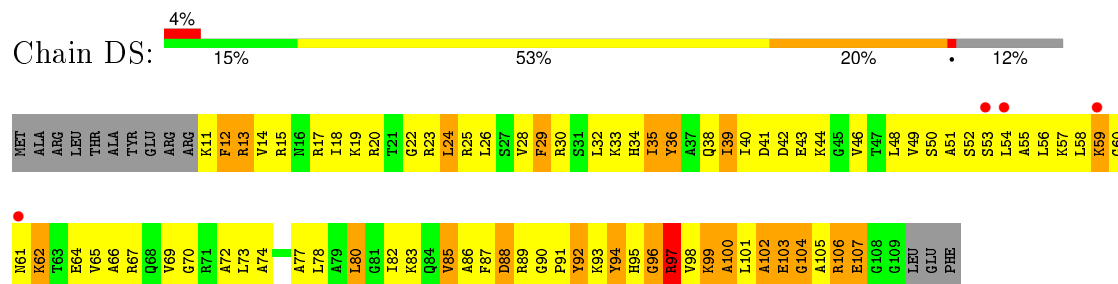
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



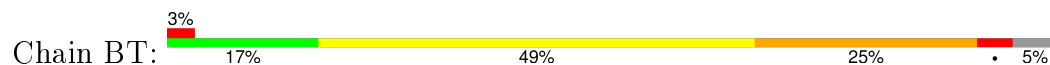
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

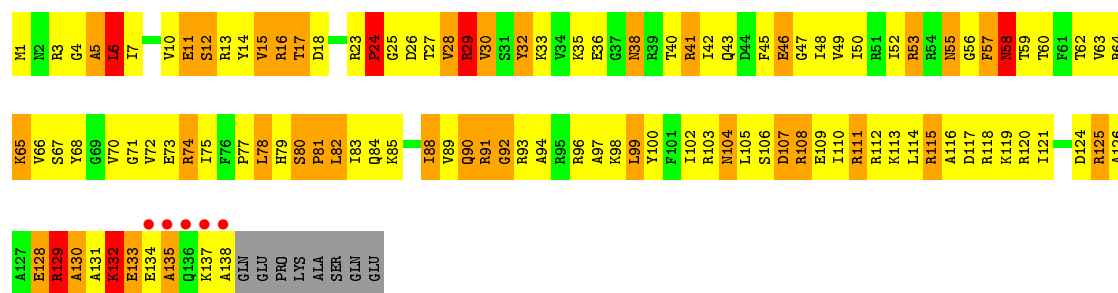


• Molecule 50: 50S RIBOSOMAL PROTEIN L18

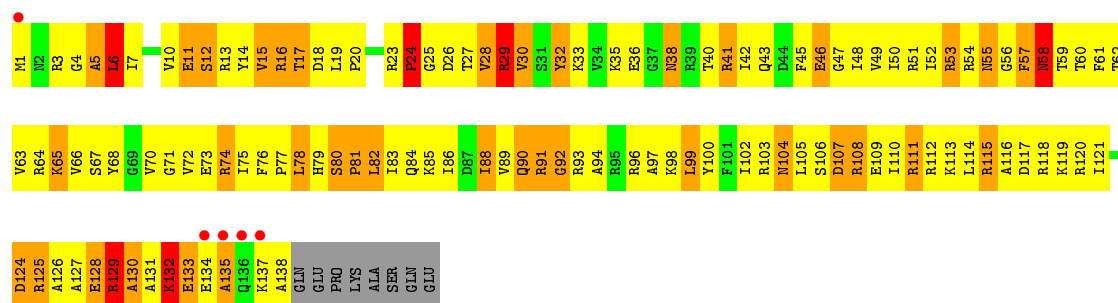
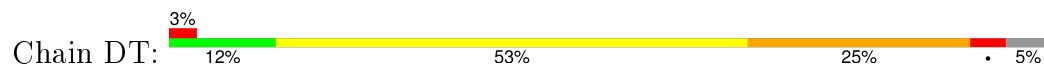


• Molecule 51: 50S RIBOSOMAL PROTEIN L19

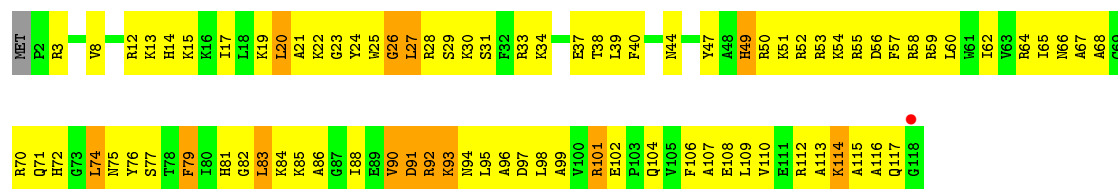




• Molecule 51: 50S RIBOSOMAL PROTEIN L19



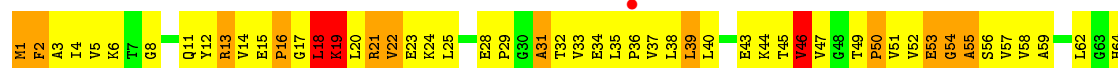
• Molecule 52: 50S RIBOSOMAL PROTEIN L20



• Molecule 52: 50S RIBOSOMAL PROTEIN L20



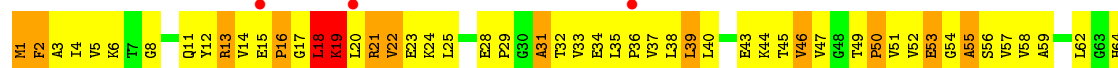
• Molecule 53: 50S RIBOSOMAL PROTEIN L21



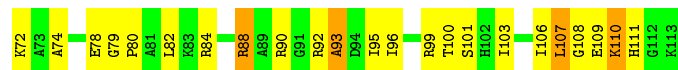
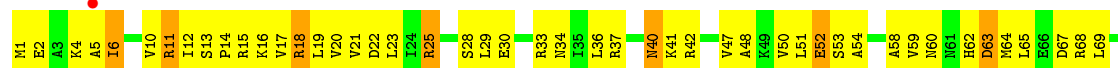
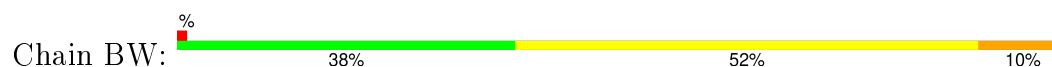




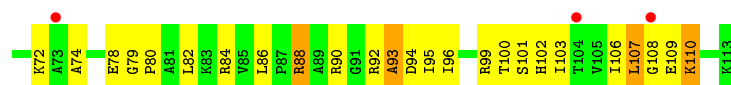
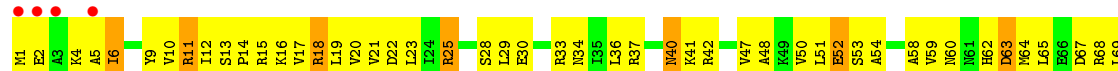
• Molecule 53: 50S RIBOSOMAL PROTEIN L21



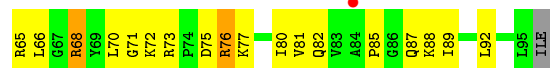
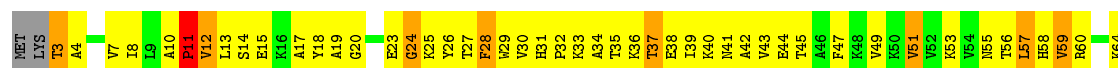
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



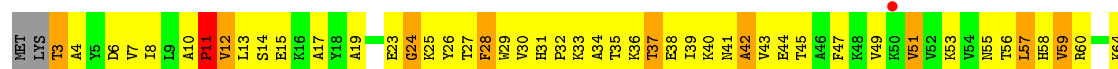
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



• Molecule 55: 50S RIBOSOMAL PROTEIN L23

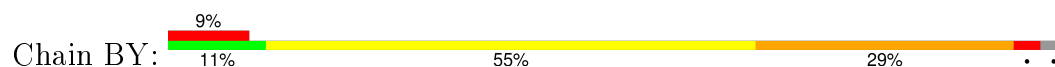


• Molecule 55: 50S RIBOSOMAL PROTEIN L23

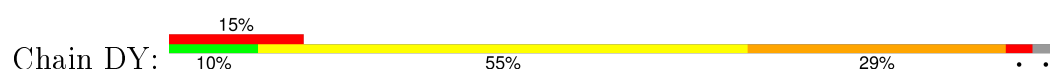




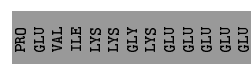
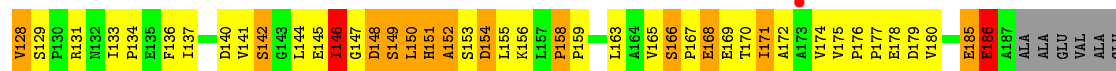
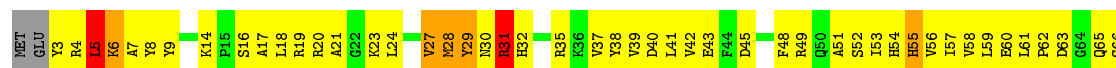
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



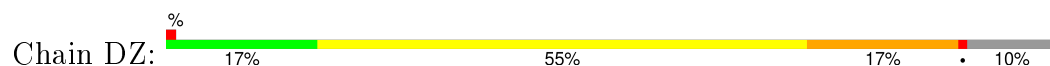
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



• Molecule 57: 50S RIBOSOMAL PROTEIN L25





## 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 0.217 , (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> )	0.28 , 96.9	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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
18	CR	574	0	644	79	0
19	AS	630	0	652	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
39	DD	2145	0	2234	315	0
40	BE	1564	0	1629	249	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

The worst 5 of 21259 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 [i](#)

### 5.3.1 Protein backbone [i](#)

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	6
2	CB	233/256 (91%)	148 (64%)	52 (22%)	33 (14%)	0	6
3	AC	205/239 (86%)	146 (71%)	32 (16%)	27 (13%)	0	6
3	CC	205/239 (86%)	148 (72%)	31 (15%)	26 (13%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	206/209 (99%)	138 (67%)	47 (23%)	21 (10%)	1	12
4	CD	206/209 (99%)	138 (67%)	49 (24%)	19 (9%)	1	15
5	AE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	4	38
5	CE	149/162 (92%)	118 (79%)	26 (17%)	5 (3%)	5	43
6	AF	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	4	38
6	CF	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	4	38
7	AG	153/156 (98%)	112 (73%)	27 (18%)	14 (9%)	1	15
7	CG	153/156 (98%)	112 (73%)	29 (19%)	12 (8%)	1	19
8	AH	136/138 (99%)	106 (78%)	26 (19%)	4 (3%)	6	46
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	6	46
9	AI	121/128 (94%)	85 (70%)	27 (22%)	9 (7%)	1	21
9	CI	121/128 (94%)	87 (72%)	25 (21%)	9 (7%)	1	21
10	AJ	97/105 (92%)	67 (69%)	19 (20%)	11 (11%)	0	9
10	CJ	97/105 (92%)	68 (70%)	18 (19%)	11 (11%)	0	9
11	AK	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	19
11	CK	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	19
12	AL	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	5
12	CL	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	5
13	AM	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	5
13	CM	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	5
14	AN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	16
14	CN	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	1	16
15	AO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	18
15	CO	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	18
16	AP	82/88 (93%)	62 (76%)	15 (18%)	5 (6%)	2	26
16	CP	82/88 (93%)	63 (77%)	14 (17%)	5 (6%)	2	26
17	AQ	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	5	45
17	CQ	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	5	45
18	AR	68/88 (77%)	47 (69%)	13 (19%)	8 (12%)	0	8
18	CR	68/88 (77%)	48 (71%)	12 (18%)	8 (12%)	0	8
19	AS	77/93 (83%)	42 (54%)	17 (22%)	18 (23%)	0	1

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	DY	105/110 (96%)	44 (42%)	32 (30%)	29 (28%)	0	0
57	BZ	183/206 (89%)	116 (63%)	39 (21%)	28 (15%)	0	5
57	DZ	183/206 (89%)	118 (64%)	34 (19%)	31 (17%)	0	4
All	All	12924/13672 (94%)	8641 (67%)	2723 (21%)	1560 (12%)	0	8

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%)	12	51
2	CB	202/220 (92%)	183 (91%)	19 (9%)	11	48
3	AC	160/188 (85%)	139 (87%)	21 (13%)	5	31
3	CC	160/188 (85%)	139 (87%)	21 (13%)	5	31
4	AD	180/181 (99%)	160 (89%)	20 (11%)	8	39
4	CD	180/181 (99%)	160 (89%)	20 (11%)	8	39
5	AE	115/123 (94%)	104 (90%)	11 (10%)	10	46
5	CE	115/123 (94%)	104 (90%)	11 (10%)	10	46
6	AF	90/90 (100%)	83 (92%)	7 (8%)	16	56
6	CF	90/90 (100%)	83 (92%)	7 (8%)	16	56
7	AG	126/127 (99%)	117 (93%)	9 (7%)	18	60
7	CG	126/127 (99%)	118 (94%)	8 (6%)	22	64
8	AH	119/119 (100%)	110 (92%)	9 (8%)	16	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	110 (92%)	9 (8%)	16	57
9	AI	98/99 (99%)	91 (93%)	7 (7%)	18	60
9	CI	98/99 (99%)	91 (93%)	7 (7%)	18	60
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	6	33
10	CJ	88/92 (96%)	76 (86%)	12 (14%)	5	30
11	AK	90/99 (91%)	87 (97%)	3 (3%)	45	79
11	CK	90/99 (91%)	87 (97%)	3 (3%)	45	79
12	AL	104/109 (95%)	93 (89%)	11 (11%)	8	42
12	CL	104/109 (95%)	93 (89%)	11 (11%)	8	42
13	AM	99/101 (98%)	90 (91%)	9 (9%)	12	49
13	CM	99/101 (98%)	90 (91%)	9 (9%)	12	49
14	AN	49/50 (98%)	44 (90%)	5 (10%)	9	43
14	CN	49/50 (98%)	44 (90%)	5 (10%)	9	43
15	AO	79/80 (99%)	73 (92%)	6 (8%)	16	57
15	CO	79/80 (99%)	73 (92%)	6 (8%)	16	57
16	AP	72/74 (97%)	68 (94%)	4 (6%)	26	68
16	CP	72/74 (97%)	68 (94%)	4 (6%)	26	68
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	28	69
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	22	64
18	AR	61/77 (79%)	58 (95%)	3 (5%)	31	71
18	CR	61/77 (79%)	58 (95%)	3 (5%)	31	71
19	AS	69/80 (86%)	60 (87%)	9 (13%)	5	32
19	CS	69/80 (86%)	60 (87%)	9 (13%)	5	32
20	AT	76/82 (93%)	66 (87%)	10 (13%)	5	31
20	CT	76/82 (93%)	67 (88%)	9 (12%)	6	36
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28	69
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	69
25	AY	563/582 (97%)	495 (88%)	68 (12%)	6	34
25	CY	563/582 (97%)	498 (88%)	65 (12%)	7	37
26	B0	66/67 (98%)	59 (89%)	7 (11%)	8	42
26	D0	66/67 (98%)	59 (89%)	7 (11%)	8	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	B1	78/83 (94%)	68 (87%)	10 (13%)	5	32
27	D1	78/83 (94%)	72 (92%)	6 (8%)	16	56
28	B2	66/67 (98%)	60 (91%)	6 (9%)	12	49
28	D2	66/67 (98%)	61 (92%)	5 (8%)	16	57
29	B3	51/52 (98%)	48 (94%)	3 (6%)	24	66
29	D3	51/52 (98%)	48 (94%)	3 (6%)	24	66
30	B4	51/63 (81%)	39 (76%)	12 (24%)	1	7
30	D4	51/63 (81%)	39 (76%)	12 (24%)	1	7
31	B5	51/52 (98%)	47 (92%)	4 (8%)	16	56
31	D5	51/52 (98%)	47 (92%)	4 (8%)	16	56
32	B6	49/52 (94%)	39 (80%)	10 (20%)	1	11
32	D6	49/52 (94%)	39 (80%)	10 (20%)	1	11
33	B7	41/42 (98%)	36 (88%)	5 (12%)	6	34
33	D7	41/42 (98%)	36 (88%)	5 (12%)	6	34
34	B8	53/55 (96%)	45 (85%)	8 (15%)	3	25
34	D8	53/55 (96%)	44 (83%)	9 (17%)	2	19
35	B9	34/34 (100%)	32 (94%)	2 (6%)	24	66
35	D9	34/34 (100%)	32 (94%)	2 (6%)	24	66
38	BC	180/181 (99%)	169 (94%)	11 (6%)	23	65
38	DC	180/181 (99%)	168 (93%)	12 (7%)	20	63
39	BD	217/218 (100%)	182 (84%)	35 (16%)	3	22
39	DD	217/218 (100%)	182 (84%)	35 (16%)	3	22
40	BE	165/166 (99%)	140 (85%)	25 (15%)	3	25
40	DE	165/166 (99%)	140 (85%)	25 (15%)	3	25
41	BF	165/166 (99%)	154 (93%)	11 (7%)	20	63
41	DF	165/166 (99%)	154 (93%)	11 (7%)	20	63
42	BG	155/156 (99%)	127 (82%)	28 (18%)	2	15
42	DG	155/156 (99%)	126 (81%)	29 (19%)	2	14
43	BH	136/148 (92%)	125 (92%)	11 (8%)	15	54
43	DH	136/148 (92%)	125 (92%)	11 (8%)	15	54
45	BN	117/119 (98%)	103 (88%)	14 (12%)	6	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DN	117/119 (98%)	103 (88%)	14 (12%)	6	35
46	BO	100/100 (100%)	94 (94%)	6 (6%)	24	66
46	DO	100/100 (100%)	94 (94%)	6 (6%)	24	66
47	BP	112/116 (97%)	93 (83%)	19 (17%)	2	19
47	DP	112/116 (97%)	92 (82%)	20 (18%)	2	16
48	BQ	111/111 (100%)	101 (91%)	10 (9%)	12	50
48	DQ	111/111 (100%)	101 (91%)	10 (9%)	12	50
49	BR	100/101 (99%)	89 (89%)	11 (11%)	8	40
49	DR	100/101 (99%)	87 (87%)	13 (13%)	5	32
50	BS	77/88 (88%)	69 (90%)	8 (10%)	9	42
50	DS	77/88 (88%)	69 (90%)	8 (10%)	9	42
51	BT	120/127 (94%)	96 (80%)	24 (20%)	1	11
51	DT	120/127 (94%)	96 (80%)	24 (20%)	1	11
52	BU	92/94 (98%)	82 (89%)	10 (11%)	8	40
52	DU	92/94 (98%)	81 (88%)	11 (12%)	6	35
53	BV	82/82 (100%)	72 (88%)	10 (12%)	6	34
53	DV	82/82 (100%)	73 (89%)	9 (11%)	8	40
54	BW	91/92 (99%)	86 (94%)	5 (6%)	27	69
54	DW	91/92 (99%)	86 (94%)	5 (6%)	27	69
55	BX	74/78 (95%)	65 (88%)	9 (12%)	6	34
55	DX	74/78 (95%)	65 (88%)	9 (12%)	6	34
56	BY	87/91 (96%)	76 (87%)	11 (13%)	5	32
56	DY	87/91 (96%)	76 (87%)	11 (13%)	5	32
57	BZ	162/179 (90%)	137 (85%)	25 (15%)	3	24
57	DZ	162/179 (90%)	145 (90%)	17 (10%)	8	42
All	All	10872/11344 (96%)	9687 (89%)	1185 (11%)	8	40

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

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Mol	Chain	Res	Type
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	12,22,23	1.32	3 (25%)	14,32,35	4.50	3 (21%)
23	5MU	CW	54	23	12,22,23	1.31	3 (25%)	14,32,35	4.48	3 (21%)

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	-	0/3/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/3/25/26	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	CW	54	5MU	C6-C5	-2.19	1.34	1.40
23	AW	54	5MU	C6-C5	-2.09	1.34	1.40
23	CW	54	5MU	C6-N1	2.21	1.38	1.35
23	AW	54	5MU	C6-N1	2.34	1.38	1.35
23	AW	54	5MU	C4-N3	2.94	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	54	5MU	C5-C4-N3	-8.93	115.20	125.14
23	CW	54	5MU	C5-C4-N3	-8.85	115.28	125.14
23	CW	54	5MU	C5M-C5-C6	2.11	122.87	118.62
23	AW	54	5MU	C5M-C5-C6	2.12	122.88	118.62
23	CW	54	5MU	C4-N3-C2	14.04	127.39	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	54	5MU	2	0
23	CW	54	5MU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	-	37,40,40	1.70	6 (16%)	45,64,64	1.66	7 (15%)
60	GDP	AY	702	61	23,30,30	1.38	3 (13%)	30,47,47	1.79	6 (20%)
59	FUA	CY	701	-	37,40,40	1.72	6 (16%)	45,64,64	1.53	7 (15%)
60	GDP	CY	702	61	23,30,30	1.46	4 (17%)	30,47,47	2.01	9 (30%)

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	-	-	0/10/92/92	0/4/4/4
60	GDP	AY	702	61	-	0/12/32/32	0/3/3/3
59	FUA	CY	701	-	-	0/10/92/92	0/4/4/4
60	GDP	CY	702	61	-	0/12/32/32	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CY	701	FUA	C23-C22	-6.14	1.39	1.51
59	AY	701	FUA	C23-C22	-5.97	1.39	1.51
59	AY	701	FUA	C23-C24	-4.18	1.39	1.53
59	CY	701	FUA	C23-C24	-4.17	1.39	1.53
59	CY	701	FUA	C24-C25	-3.98	1.39	1.50

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AY	702	GDP	C5-C6-N1	-4.67	117.20	123.59
60	AY	702	GDP	N3-C2-N1	-4.58	120.47	127.44
60	CY	702	GDP	N3-C2-N1	-4.56	120.50	127.44
59	AY	701	FUA	C13-C12-C11	-4.51	105.84	111.95
60	CY	702	GDP	PA-O3A-PB	-4.07	119.01	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AY	701	FUA	15	0
60	AY	702	GDP	13	0
59	CY	701	FUA	26	0
60	CY	702	GDP	10	0

## 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
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%)	-0.00	38 (2%) 61 45	34, 72, 165, 200	0
1	CA	1504/1522 (98%)	0.00	30 (1%) 68 53	43, 89, 174, 200	0
2	AB	235/256 (91%)	-0.44	1 (0%) 93 88	40, 82, 172, 191	0
2	CB	235/256 (91%)	-0.26	1 (0%) 93 88	53, 102, 164, 194	0
3	AC	207/239 (86%)	-0.57	0 100 100	23, 69, 122, 174	0
3	CC	207/239 (86%)	-0.46	0 100 100	45, 93, 143, 190	0
4	AD	208/209 (99%)	-0.27	0 100 100	46, 95, 144, 166	0
4	CD	208/209 (99%)	-0.20	1 (0%) 91 86	48, 107, 157, 188	0
5	AE	151/162 (93%)	-0.45	2 (1%) 79 66	27, 62, 107, 187	0
5	CE	151/162 (93%)	-0.31	3 (1%) 68 53	45, 76, 117, 200	0
6	AF	101/101 (100%)	-0.46	0 100 100	44, 85, 125, 174	0
6	CF	101/101 (100%)	-0.06	2 (1%) 68 53	72, 115, 152, 183	0
7	AG	155/156 (99%)	-0.42	1 (0%) 90 83	36, 80, 126, 182	0
7	CG	155/156 (99%)	-0.23	3 (1%) 70 55	63, 108, 150, 193	0
8	AH	138/138 (100%)	-0.53	0 100 100	35, 65, 111, 136	0
8	CH	138/138 (100%)	-0.42	0 100 100	45, 79, 117, 147	0
9	AI	127/128 (99%)	-0.20	0 100 100	41, 79, 135, 157	0
9	CI	127/128 (99%)	-0.02	2 (1%) 74 60	68, 111, 151, 175	0
10	AJ	99/105 (94%)	-0.01	4 (4%) 42 28	33, 87, 180, 193	0
10	CJ	99/105 (94%)	0.20	2 (2%) 68 53	60, 127, 179, 190	0
11	AK	119/129 (92%)	-0.26	3 (2%) 61 45	27, 62, 109, 171	0
11	CK	119/129 (92%)	-0.07	3 (2%) 61 45	48, 89, 126, 181	0
12	AL	125/132 (94%)	-0.31	3 (2%) 62 46	37, 76, 118, 180	0
12	CL	125/132 (94%)	-0.09	3 (2%) 62 46	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%)	0.03	5 (4%) 42 28	52, 98, 165, 200	0
13	CM	125/126 (99%)	0.18	7 (5%) 28 18	63, 126, 171, 200	0
14	AN	60/61 (98%)	-0.38	0 100 100	35, 62, 103, 131	0
14	CN	60/61 (98%)	-0.19	1 (1%) 73 58	58, 91, 127, 146	0
15	AO	88/89 (98%)	-0.45	0 100 100	27, 71, 116, 144	0
15	CO	88/89 (98%)	-0.29	0 100 100	31, 82, 119, 141	0
16	AP	84/88 (95%)	-0.13	0 100 100	36, 85, 130, 160	0
16	CP	84/88 (95%)	0.01	0 100 100	58, 95, 126, 166	0
17	AQ	100/105 (95%)	-0.30	0 100 100	40, 78, 112, 139	0
17	CQ	100/105 (95%)	-0.18	0 100 100	60, 84, 120, 147	0
18	AR	70/88 (79%)	-0.35	1 (1%) 78 64	38, 72, 119, 167	0
18	CR	70/88 (79%)	-0.25	1 (1%) 78 64	60, 95, 142, 167	0
19	AS	79/93 (84%)	-0.12	1 (1%) 79 66	63, 95, 174, 182	0
19	CS	79/93 (84%)	0.26	3 (3%) 44 30	74, 117, 181, 199	0
20	AT	99/106 (93%)	0.07	1 (1%) 84 72	55, 95, 147, 176	0
20	CT	99/106 (93%)	0.03	1 (1%) 84 72	72, 103, 153, 173	0
21	AU	25/27 (92%)	0.20	2 (8%) 15 9	33, 84, 132, 167	0
21	CU	25/27 (92%)	0.60	2 (8%) 15 9	77, 115, 145, 164	0
22	AV	76/76 (100%)	-0.01	1 (1%) 79 66	51, 94, 154, 200	0
22	CV	76/76 (100%)	0.01	2 (2%) 59 43	67, 107, 165, 200	0
23	AW	76/77 (98%)	0.76	9 (11%) 6 5	97, 182, 200, 200	0
23	CW	76/77 (98%)	0.86	9 (11%) 6 5	97, 190, 200, 200	0
24	AX	12/25 (48%)	2.62	8 (66%) 0 1	52, 114, 167, 193	0
24	CX	12/25 (48%)	2.18	5 (41%) 0 1	52, 114, 172, 193	0
25	AY	667/691 (96%)	0.57	77 (11%) 6 5	71, 142, 179, 200	0
25	CY	667/691 (96%)	0.69	94 (14%) 4 3	84, 151, 186, 200	0
26	B0	84/85 (98%)	0.21	3 (3%) 46 32	61, 87, 134, 191	0
26	D0	84/85 (98%)	0.71	8 (9%) 10 6	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%)	0.13	3 (3%) 51 35	59, 99, 153, 181	0
28	B2	71/72 (98%)	0.06	3 (4%) 40 27	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%)	0.28	2 (2%) 56 41	82, 134, 172, 186	0
29	B3	60/60 (100%)	0.55	5 (8%) 14 9	55, 95, 148, 180	0
29	D3	60/60 (100%)	0.48	2 (3%) 50 35	61, 105, 145, 174	0
30	B4	58/71 (81%)	0.26	2 (3%) 49 34	90, 141, 200, 200	0
30	D4	58/71 (81%)	0.28	3 (5%) 31 21	106, 166, 200, 200	0
31	B5	59/60 (98%)	-0.01	3 (5%) 32 21	46, 96, 175, 192	0
31	D5	59/60 (98%)	0.11	3 (5%) 32 21	50, 104, 167, 200	0
32	B6	50/54 (92%)	0.42	4 (8%) 15 9	55, 97, 142, 173	0
32	D6	50/54 (92%)	0.53	3 (6%) 25 15	71, 111, 153, 178	0
33	B7	49/49 (100%)	0.08	1 (2%) 68 53	51, 79, 117, 200	0
33	D7	49/49 (100%)	0.03	0 100 100	64, 91, 127, 166	0
34	B8	64/65 (98%)	-0.10	2 (3%) 52 37	51, 81, 124, 148	0
34	D8	64/65 (98%)	0.06	1 (1%) 74 60	67, 104, 137, 168	0
35	B9	37/37 (100%)	0.09	2 (5%) 29 19	66, 89, 127, 141	0
35	D9	37/37 (100%)	0.27	2 (5%) 29 19	65, 91, 151, 187	0
36	BA	2901/2915 (99%)	0.06	62 (2%) 67 52	36, 88, 184, 200	0
36	DA	2901/2915 (99%)	0.07	63 (2%) 65 50	42, 102, 186, 200	0
37	BB	119/122 (97%)	-0.23	1 (0%) 87 77	68, 101, 129, 160	0
37	DB	119/122 (97%)	-0.15	0 100 100	83, 126, 154, 189	0
38	BC	228/229 (99%)	-0.10	6 (2%) 59 43	44, 101, 163, 195	0
38	DC	228/229 (99%)	0.25	13 (5%) 27 17	66, 125, 187, 199	0
39	BD	275/276 (99%)	-0.39	1 (0%) 93 88	31, 64, 106, 155	0
39	DD	275/276 (99%)	-0.36	0 100 100	40, 74, 115, 163	0
40	BE	205/206 (99%)	-0.12	2 (0%) 84 72	37, 88, 146, 184	0
40	DE	205/206 (99%)	-0.05	3 (1%) 76 62	50, 97, 157, 200	0
41	BF	208/210 (99%)	-0.05	5 (2%) 62 46	53, 111, 183, 200	0
41	DF	208/210 (99%)	0.15	8 (3%) 44 30	58, 131, 186, 200	0
42	BG	181/182 (99%)	-0.28	4 (2%) 65 50	51, 99, 144, 194	0
42	DG	181/182 (99%)	-0.04	5 (2%) 56 41	67, 122, 168, 192	0
43	BH	167/180 (92%)	0.48	9 (5%) 29 19	87, 131, 174, 185	0
43	DH	167/180 (92%)	0.36	5 (2%) 54 37	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%)	-0.19	0 100 100	60, 99, 148, 177	0
45	DN	139/140 (99%)	-0.07	3 (2%) 65 50	64, 108, 162, 176	0
46	BO	122/122 (100%)	-0.26	0 100 100	34, 72, 107, 128	0
46	DO	122/122 (100%)	-0.26	0 100 100	40, 79, 108, 156	0
47	BP	146/150 (97%)	0.17	2 (1%) 78 64	48, 104, 158, 195	0
47	DP	146/150 (97%)	0.54	7 (4%) 34 22	52, 127, 173, 195	0
48	BQ	141/141 (100%)	-0.31	0 100 100	39, 77, 122, 173	0
48	DQ	141/141 (100%)	-0.26	1 (0%) 89 81	52, 86, 127, 185	0
49	BR	117/118 (99%)	-0.16	0 100 100	36, 89, 128, 177	0
49	DR	117/118 (99%)	-0.04	0 100 100	46, 95, 135, 181	0
50	BS	99/112 (88%)	-0.12	1 (1%) 84 72	53, 109, 156, 191	0
50	DS	99/112 (88%)	0.36	4 (4%) 42 28	51, 121, 164, 192	0
51	BT	138/146 (94%)	-0.19	5 (3%) 46 32	53, 95, 168, 200	0
51	DT	138/146 (94%)	-0.19	5 (3%) 46 32	56, 103, 172, 200	0
52	BU	117/118 (99%)	-0.29	1 (0%) 85 75	55, 91, 138, 200	0
52	DU	117/118 (99%)	-0.19	1 (0%) 85 75	66, 104, 147, 191	0
53	BV	101/101 (100%)	0.02	2 (1%) 68 53	43, 112, 158, 177	0
53	DV	101/101 (100%)	0.34	4 (3%) 42 28	64, 126, 171, 193	0
54	BW	113/113 (100%)	-0.01	1 (0%) 85 75	56, 95, 150, 195	0
54	DW	113/113 (100%)	0.30	7 (6%) 24 14	73, 106, 158, 194	0
55	BX	93/96 (96%)	-0.07	1 (1%) 82 70	61, 101, 133, 176	0
55	DX	93/96 (96%)	-0.03	1 (1%) 82 70	63, 111, 141, 154	0
56	BY	107/110 (97%)	0.69	10 (9%) 11 7	93, 138, 178, 187	0
56	DY	107/110 (97%)	1.13	16 (14%) 3 2	87, 147, 182, 200	0
57	BZ	185/206 (89%)	-0.02	2 (1%) 82 70	50, 108, 163, 190	0
57	DZ	185/206 (89%)	0.11	2 (1%) 82 70	54, 122, 170, 199	0
All	All	22516/23492 (95%)	0.02	647 (2%) 55 39	23, 98, 175, 200	0

The worst 5 of 647 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	DA	654(E)	G	13.5
1	AA	89	C	12.6
23	CW	17	C	12.0
36	DA	654(D)	G	11.6
36	BA	654(D)	G	11.4

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	5MU	AW	54	21/22	0.58	0.27	-	200,200,200,200	0
23	5MU	CW	54	21/22	0.79	0.15	-	200,200,200,200	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
59	FUA	AY	701	37/37	0.68	0.65	2.76	98,102,110,111	0
58	ZN	AD	301	1/1	0.98	0.30	1.81	78,78,78,78	0
59	FUA	CY	701	37/37	0.62	0.64	1.66	102,104,107,109	0
58	ZN	AN	101	1/1	0.97	0.24	1.28	84,84,84,84	0
60	GDP	AY	702	28/28	0.88	0.23	-0.27	93,97,99,99	0
58	ZN	CD	301	1/1	0.99	0.23	-0.28	69,69,69,69	0
60	GDP	CY	702	28/28	0.92	0.17	-1.15	96,102,109,110	0
58	ZN	CN	101	1/1	0.99	0.14	-1.17	86,86,86,86	0
58	ZN	B9	101	1/1	0.99	0.10	-1.31	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	ZN	D4	1000	1/1	0.34	0.14	-1.33	200,200,200,200	0
58	ZN	D9	1000	1/1	0.96	0.09	-1.48	123,123,123,123	0
58	ZN	B4	101	1/1	0.91	0.08	-3.39	172,172,172,172	0
61	MG	AY	703	1/1	0.97	0.31	-	55,55,55,55	0
61	MG	CY	703	1/1	0.87	0.22	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.