



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:23 PM BST

PDB ID : 4V5L
Title : The structure of EF-Tu and aminoacyl-tRNA bound to the 70S ribosome with a GTP analog
Authors : Voorhees, R.M.; Schmeing, T.M.; Ramakrishnan, V.
Deposited on : 2010-09-02
Resolution : 3.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

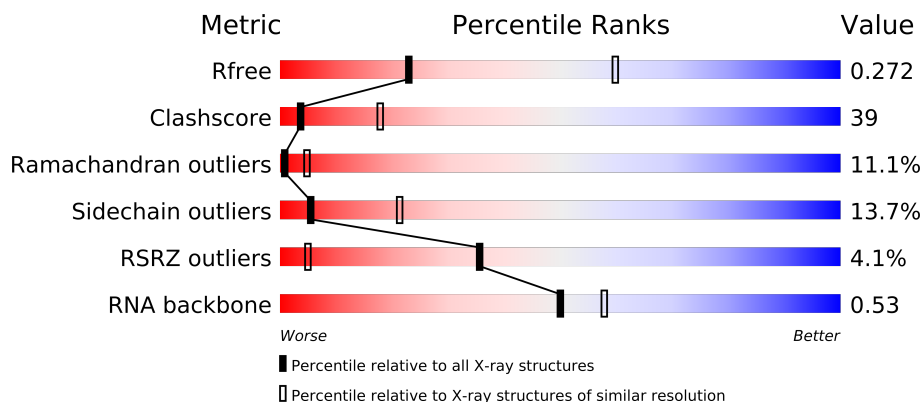
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	AB	256	
3	AC	239	
4	AD	209	
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	

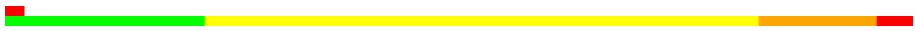
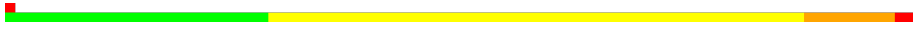

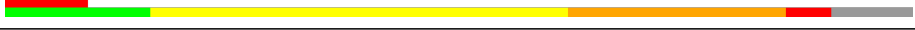
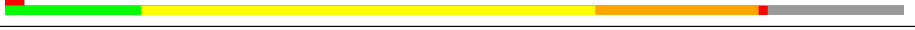
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Mol	Chain	Length	Quality of chain
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	76	
22	AW	76	
23	AX	14	
24	AY	77	
25	AZ	405	
26	B0	85	
27	B1	98	
28	B2	72	
29	B3	60	
30	B4	71	
31	B5	60	
32	B6	54	
33	B7	49	
34	B8	65	
35	B9	37	
36	BA	2915	
37	BB	122	
38	BC	229	
39	BD	276	
40	BE	206	
41	BF	210	
42	BG	182	
43	BH	180	
44	BJ	130	
45	BK	140	
46	BN	140	
47	BO	122	
48	BP	150	
49	BQ	141	
50	BR	118	
51	BS	112	
52	BT	146	
53	BU	118	

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Mol	Chain	Length	Quality of chain
54	BV	101	
55	BW	113	
56	BX	96	
57	BY	110	
58	BZ	206	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 153628 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

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

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

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

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

- 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			

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

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

- 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			

- 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			

- 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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

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

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

- 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			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	EXPRESSION TAG	UNP P17293
AL	2	VAL	-	EXPRESSION TAG	UNP P17293
AL	3	ALA	-	EXPRESSION TAG	UNP P17293
AL	4	LEU	-	EXPRESSION TAG	UNP P17293

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- 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			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- 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			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	14	Total	C	N	O	P	0	0	0
			298	135	56	94	13			

- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

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

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	405	Total	C	N	O	S	0	0	0
			3142	1983	550	597	12			

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

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

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

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

- 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			

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

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

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

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

- 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			

- 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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- 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			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

- 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			

- 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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	27	ARG	LEU	CONFLICT	UNP Q5SLP7

- 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			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- 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			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O		0	0	0
			651	391	130	130				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O		0	0	0
			700	420	140	140				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	98	Total	C	N	O	S	0	0	0
			770	486	154	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

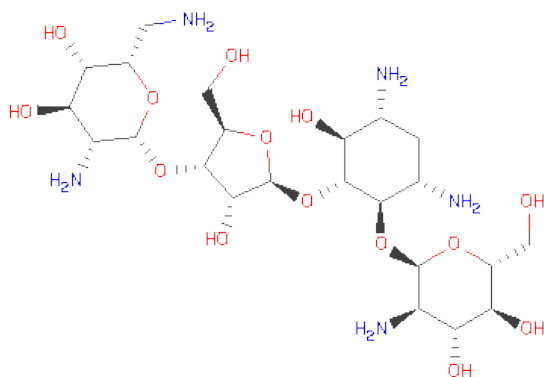
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

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

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

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).

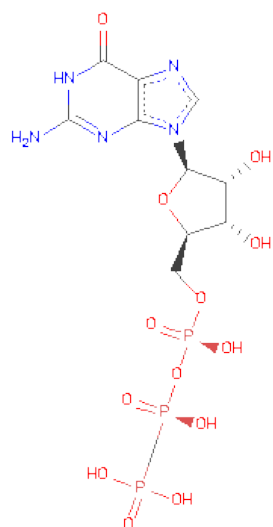


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B9	1	Total	Zn	0	0
			1	1		
60	B4	1	Total	Zn	0	0
			1	1		
60	AD	1	Total	Zn	0	0
			1	1		
60	AN	1	Total	Zn	0	0
			1	1		

- Molecule 61 is PHOSPHOMETHYLPHOSPHONICACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



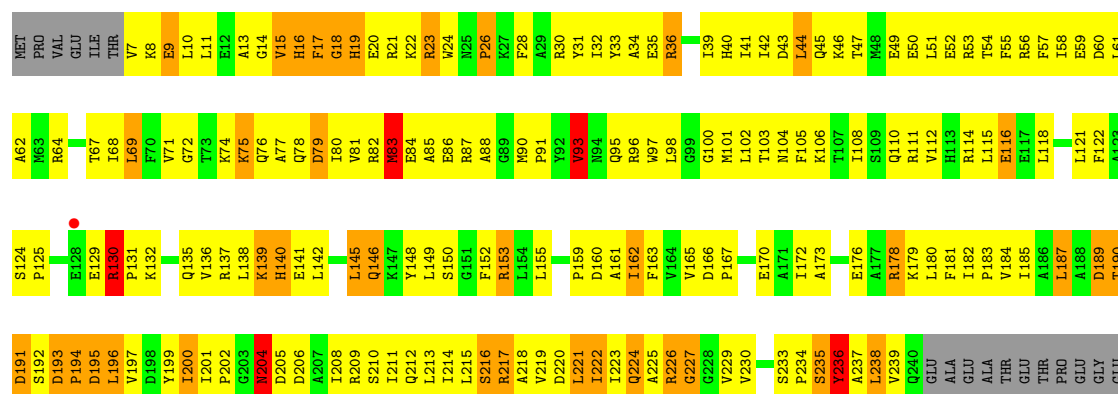
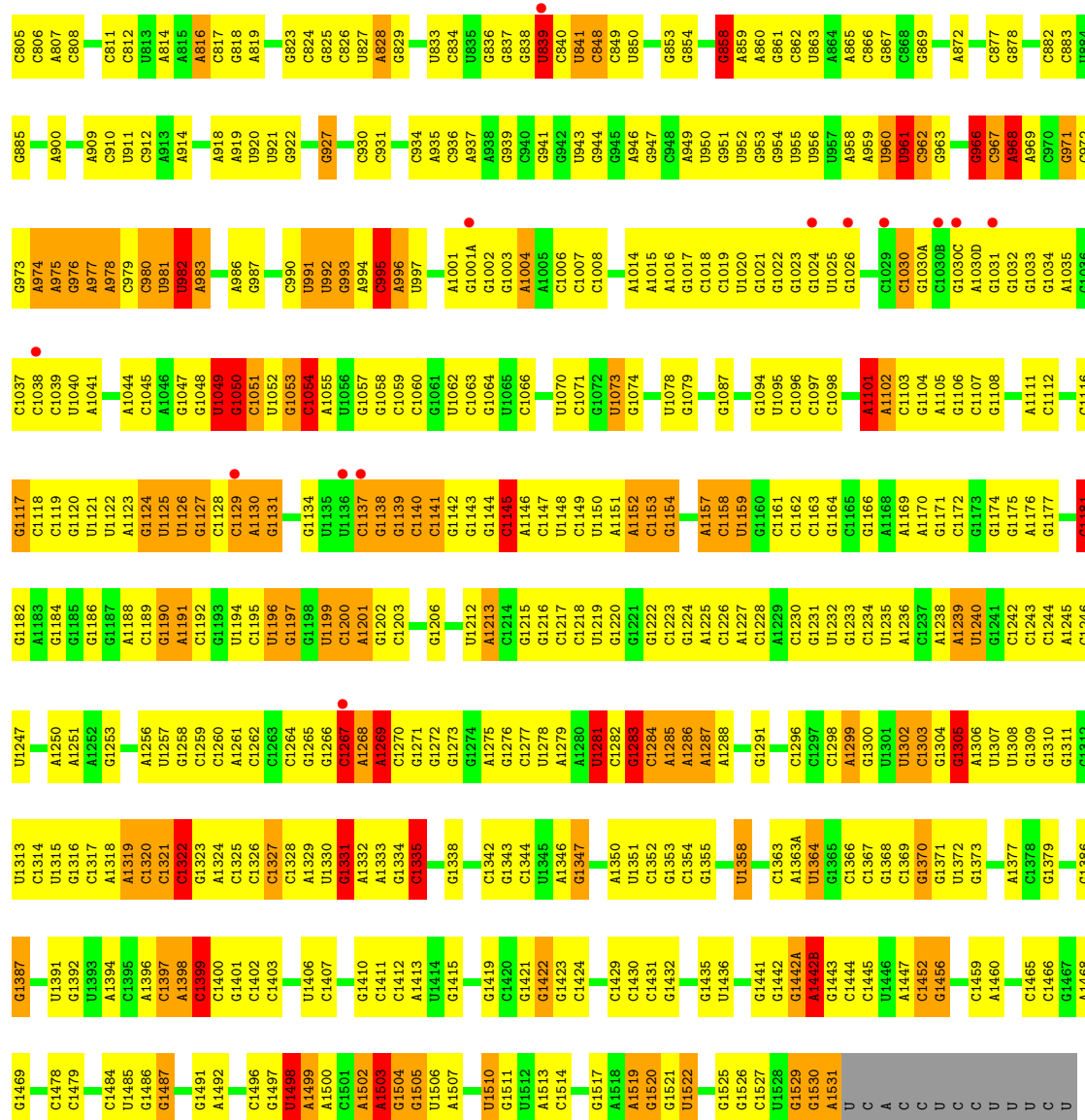
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AZ	1	Total	Mg	0	0
			1	1		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AZ	1	Total	O	0	0
			1	1		



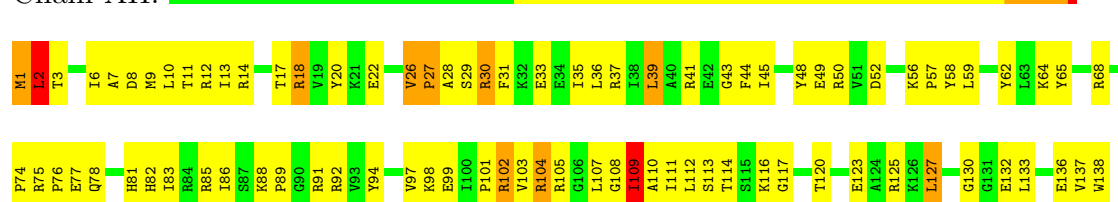
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



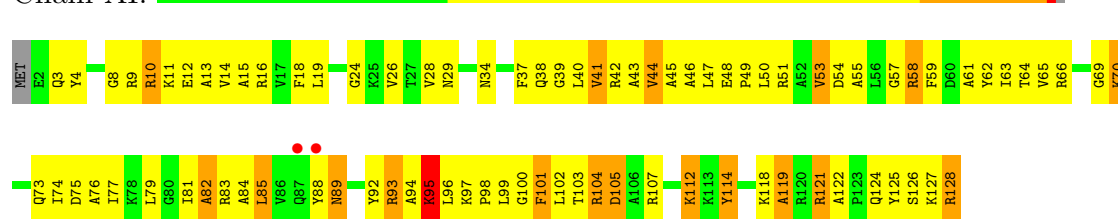
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



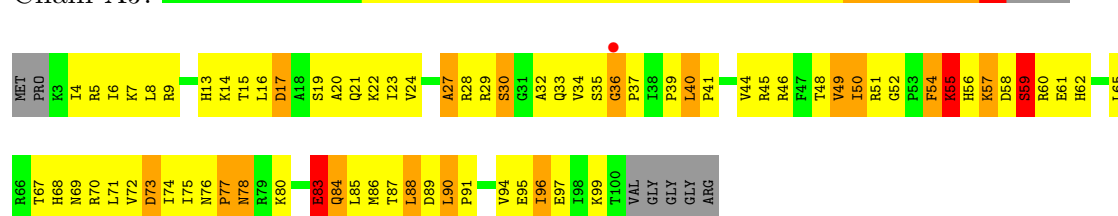
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



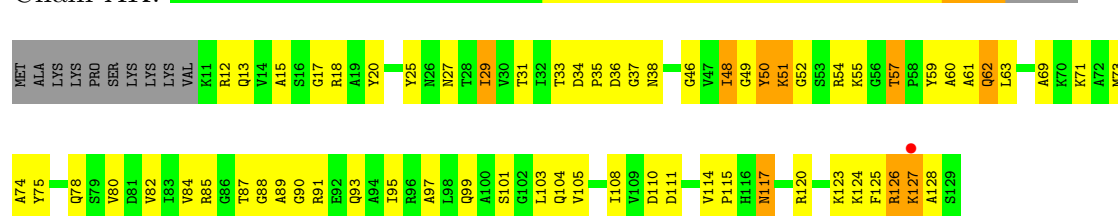
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



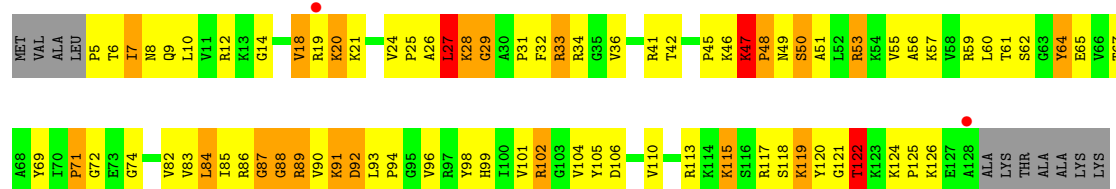
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



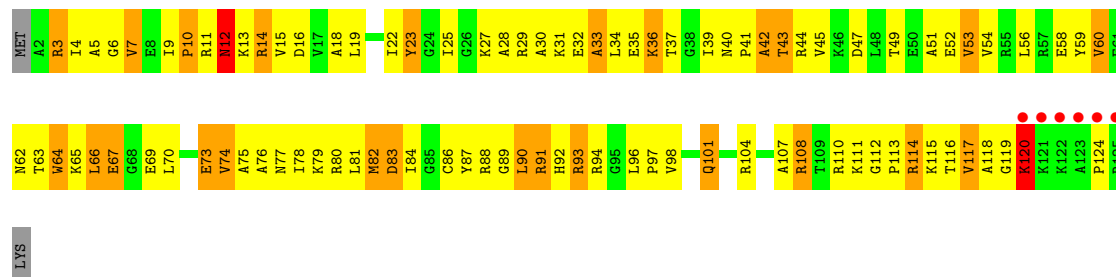
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



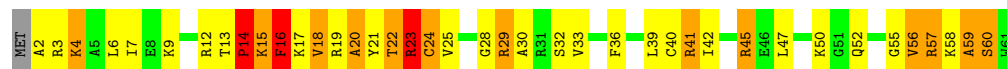
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



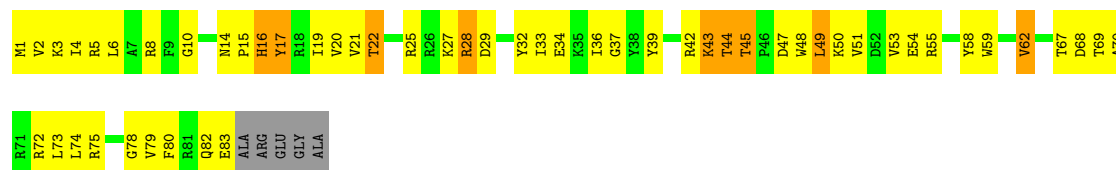
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



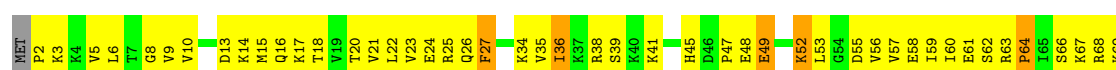
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

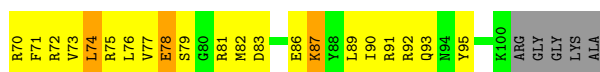
Chain AP:



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

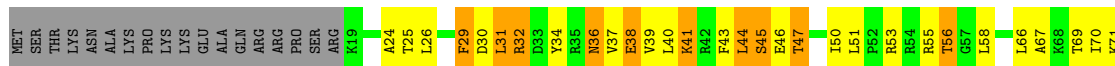
Chain AQ:





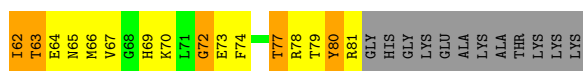
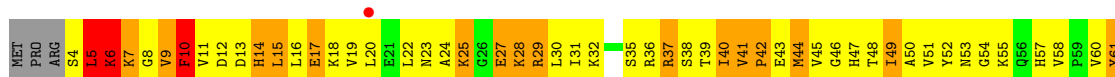
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



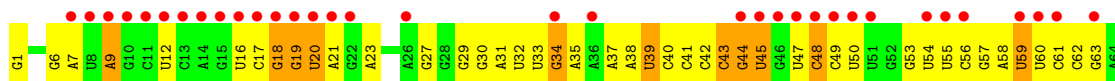
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

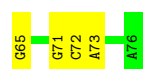
Chain AV:



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

Chain AW:





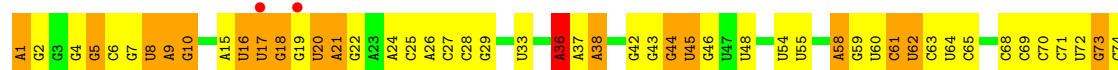
- Molecule 23: MRNA

Chain AX:



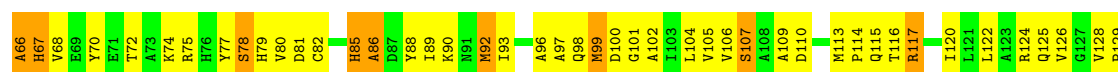
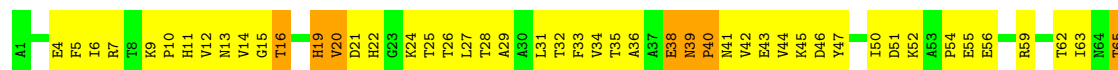
- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

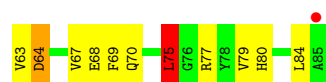
Chain AY:



- Molecule 25: ELONGATION FACTOR TU

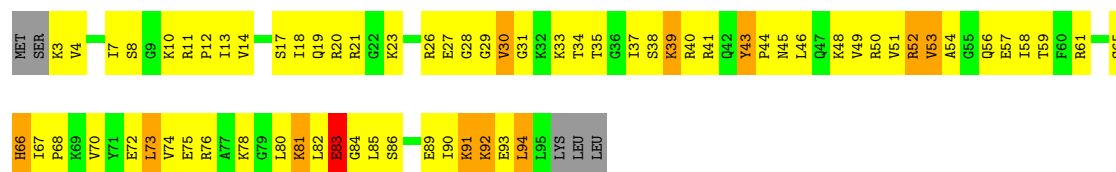
Chain AZ:





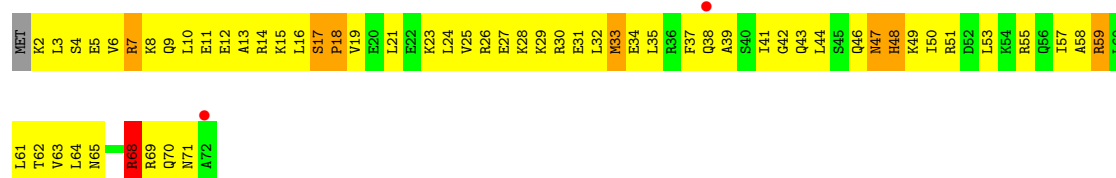
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



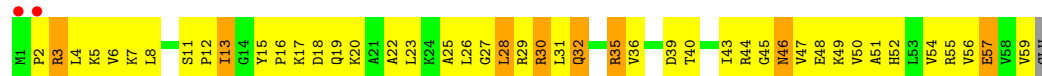
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



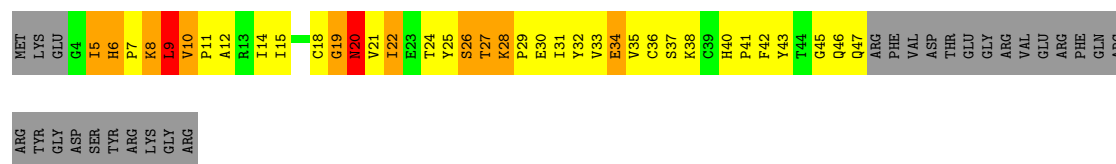
• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



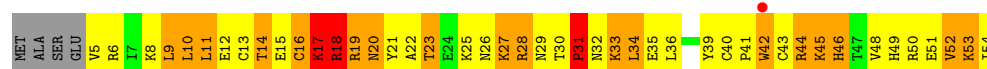
• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5:



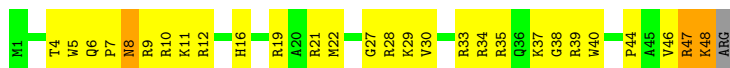
• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:



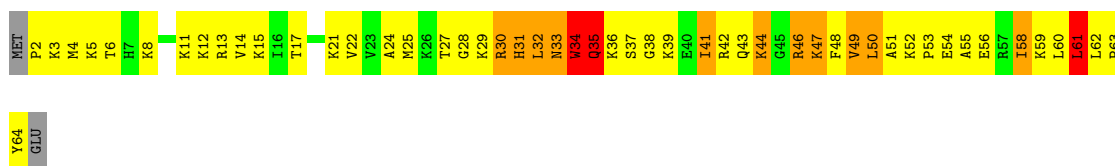
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:



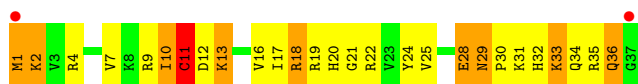
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



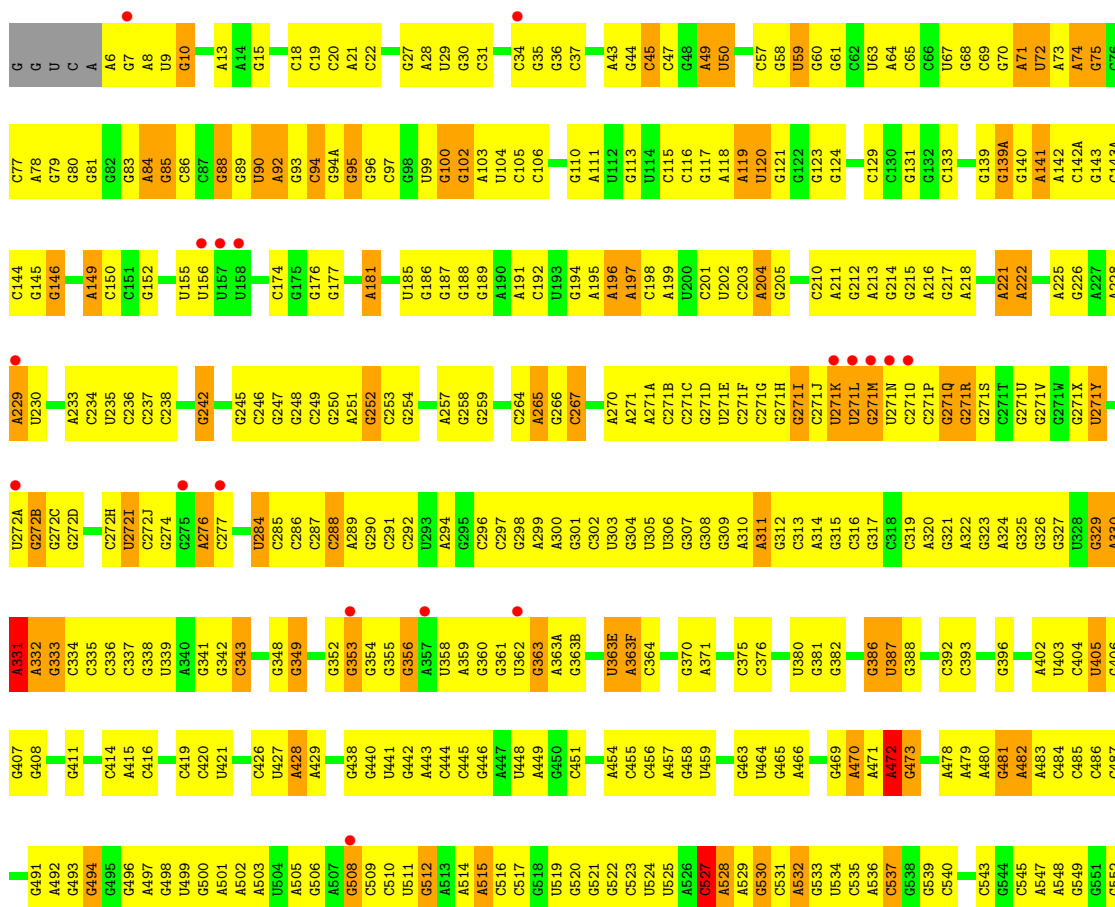
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



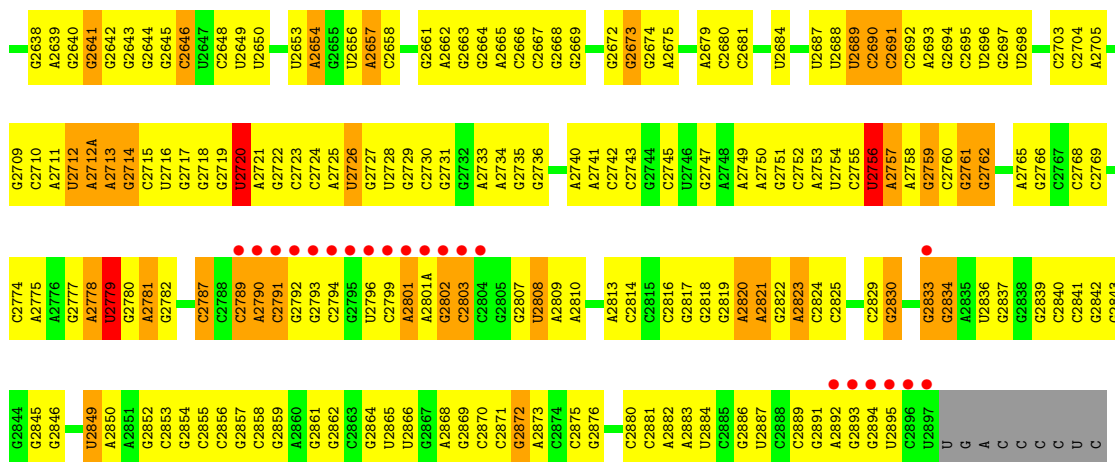
- Molecule 36: 23S RIBOSOMAL RNA

Chain BA:



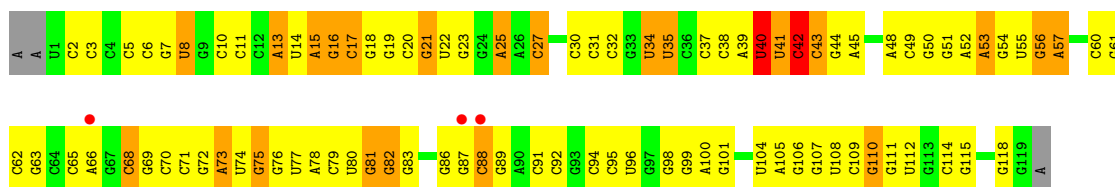
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A1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	A1445	C1445A	C1446	G1447	G1448	G1449	G1450	C1450A	G1451	A1452	G1453	G1455	G1458	G1459	G1460	G1461	C1462	C1463	G1464	C1467	C1468	A1469	G1470	A1471	G1472	G1473	G1474	G1475	G1478	G1479	G1480	G1481	G1482																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A1342	G1343	G1344	G1348	G1349	G1350	C1351	G1352	A1353	A1354	G1355	A1359	A1360	G1361	C1362	C1363	C1364	A1365	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	A1378	A1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	A1395	U1396	U1397	C1398	C1399	G1400	G1401	G1402	G1403	A1404	U1405	U1406	G1407	C1408	G1409	G1410	C1411																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U1273	A1274	A1275	A1278	G1279	G1285	A1286	A1287	U1288	G1289	C1290	C1291	U1292	C1293	G1296	G1297	G1298	G1299	U1300	A1301	A1302	C1303	C1304	C1305	A1308	G1309	G1310	G1311	U1312	U1313	C1314	C1315	U1316	A1317	G1318	G1319	C1320	A1321	G1324	C1327	G1328	U1329	C1330	A1331	G1332	C1333	G1334	U1335	A1336	U1337	G1338	U1339	U1340	U1341																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U1211	G1212	A1213	A1214	G1215	G1216	C1217	G1218	G1219	A1220	C1221	G1222	G1223	C1224	G1225	A1226	G1227	G1228	G1229	C1230	G1231	G1232	G1233	U1234	G1235	G1238	U1239	U1240	A1241	A1242	G1243	G1244	A1245	A1246	A1247	G1248	C1251	G1252	A1253	U1254	U1255	G1256	C1257	G1258	G1259	G1260	U1263	G1264	A1265	G1266	U1267	A1268	A1269	G1270	U1271	A1272																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C1145	A1148	G1149	C1150	G1151	C1152	C1153	G1154	A1155	A1156	C1157	G1158	U1159	G1160	C1161	G1162	G1163	G1164	U1165	C1166	U1167	G1168	G1169	G1170	G1171	G1173	U1174	U1175	G1176	A1177	C1178	G1179	C1180	G1184	C1185	G1186	G1187	U1188	A1189	G1190	G1191	G1192	G1193	A1194	G1195	U1198	U1199	C1202	G1203	A1204	U1205	U1206	G1207	C1208	G1209	A1210																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U1082	U1083	A1084	A1085	A1086	G1087	A1088	G1089	U1090	G1091	C1092	G1093	U1094	A1095	U1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	G1115	C1116	A1057	G1058	G1059	C1121	G1122	C1123	C1124	G1125	A1129	U1130	G1131	A1132	U1133	G1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	A1142A	G1143	G1144																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C1018	U1019	A1020	A1021	G1022	G1023	G1024	G1025	U1026	A1027	A1028	A1032	U1033	G1034	C1038	G1039	C1040	G1041	G1042	C1043	G1044	A1045	A1046	G1047	C1048	A1049	A1050	G1051	C1052	C1053	A1054	G1055	C985	C986	G987	A988	G989	A990	C991	C995	A996	G997	C998	U999	A1000	A1001	G1002	C1005	C1006	U1007	A1010	G1011	U1012	U1013	U1014	U1081																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A945	G946	G947	G948	C949	G950	G951	G952	C955	A957	U958	A959	A960	A961	U963	C964	C965	G968	U969	G970	U971	G972	A973	A974	C975	A981	A983	A984	C985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	G1002	C1005	C1006	U1007	A1010	G1011	U1012	U1013	U1014	U1081																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G880	G881	G882	G883	C884	G885	C886	A887	C888	A889	C890	C891	C892	C893	C894	U895	C897	C898	C899	C900	A909	A910	A911	C912	U913	C914	C915	A916	A917	A918	A919	A920	G921	U922	C923	C924	C925	A926	G927	C928	G932	A933	G934	C935	C936	U937	G938	G939	G940	A941	G942	U943	G944																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A804	G805	C806	U807	U810	U811	C812	U813	U814	C815	A819	A820	A821	U822	U827	U828	A829	G831	G832	U833	C834	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	G869	G870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530</





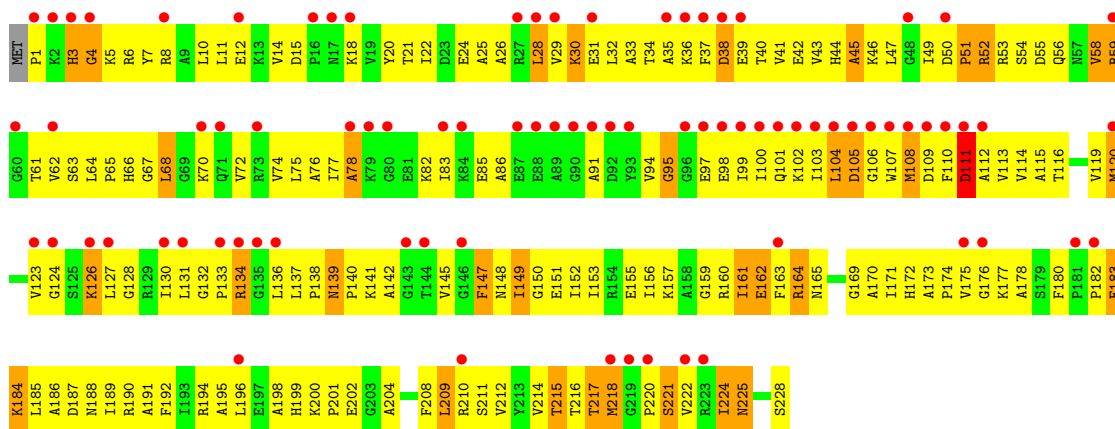
• Molecule 37: 5S RIBOSOMAL RNA

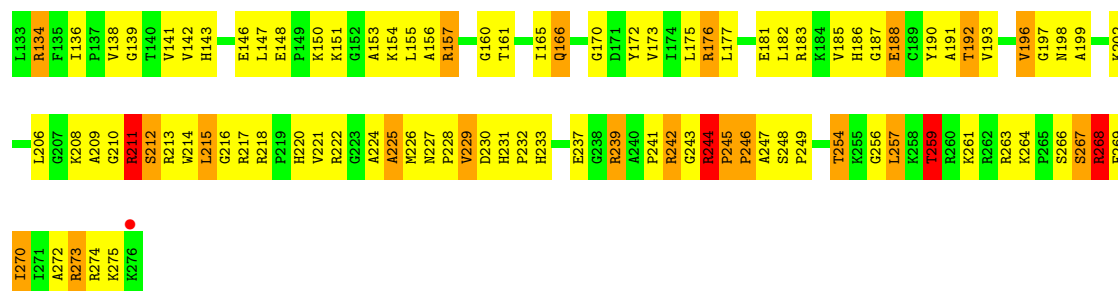
Chain BB:



• Molecule 38: 50S RIBOSOMAL PROTEIN L1

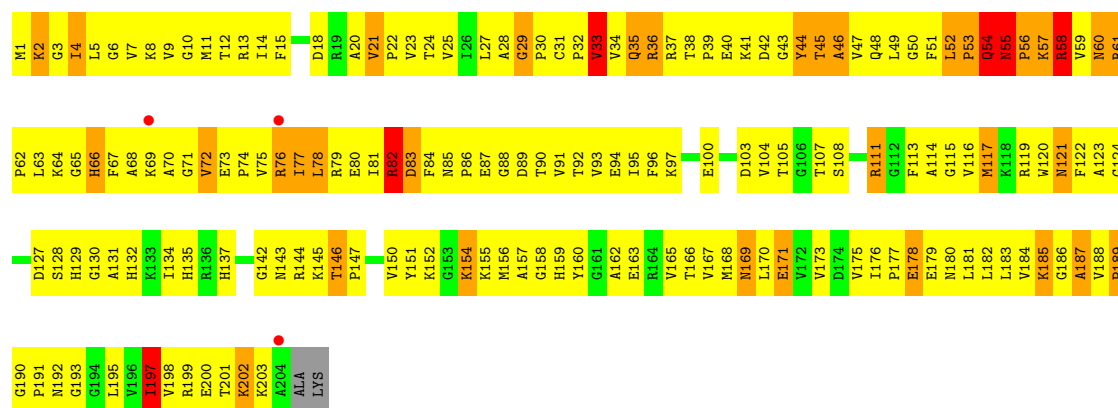
Chain BC:





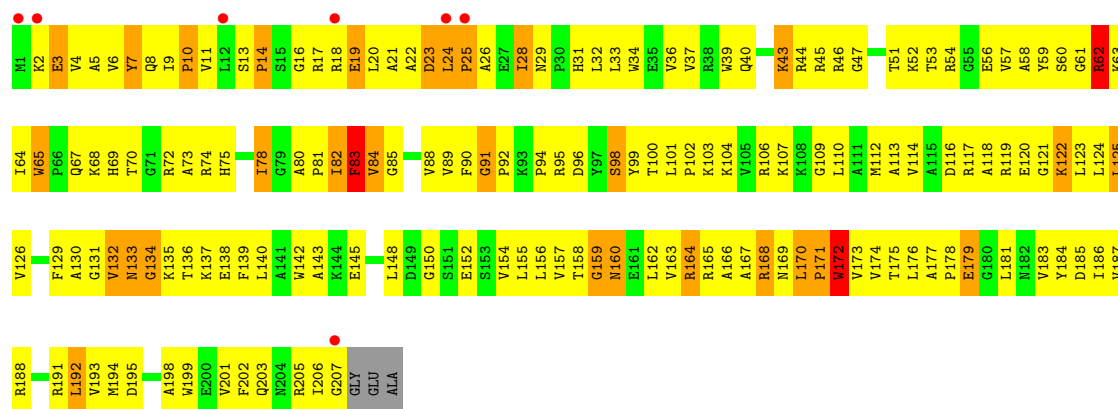
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain BE:



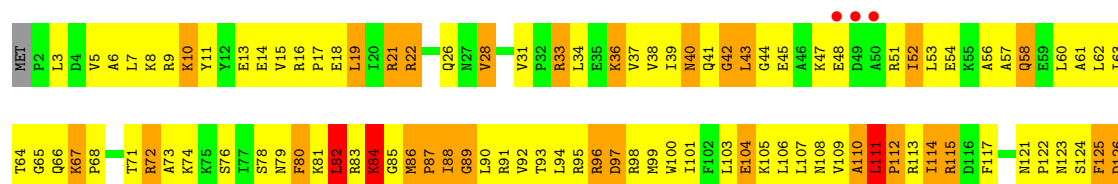
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF:



• Molecule 42: 50S RIBOSOMAL PROTEIN L5

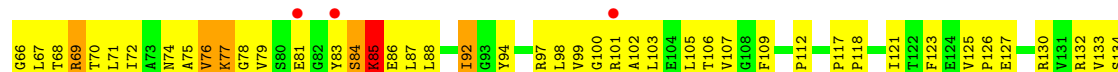
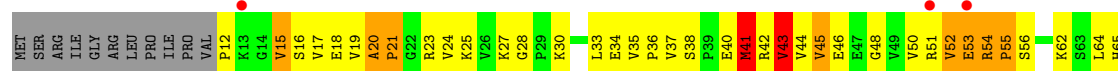
Chain BG:





• Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain BH:



• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



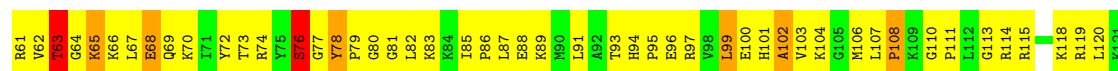
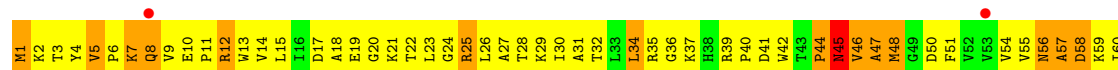
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

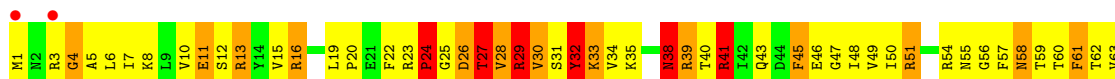
Chain BN:

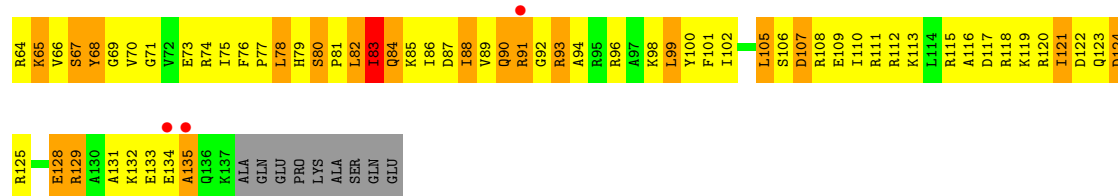


• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:

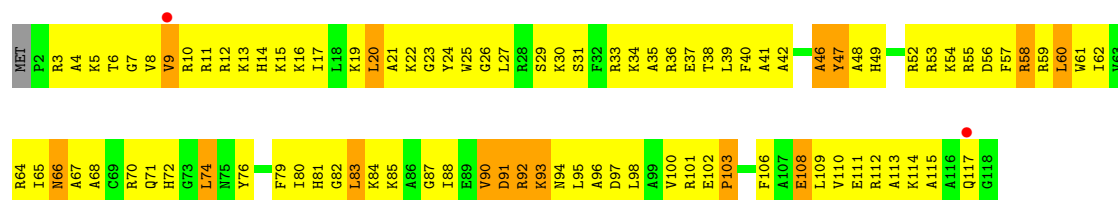






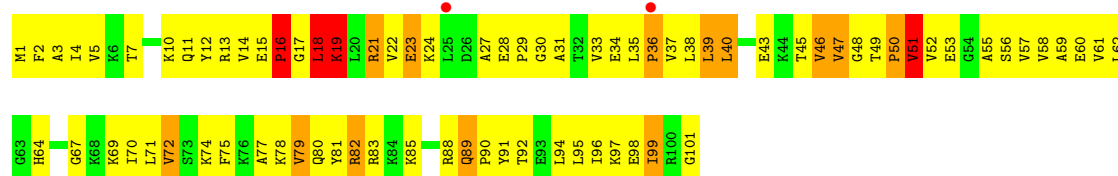
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



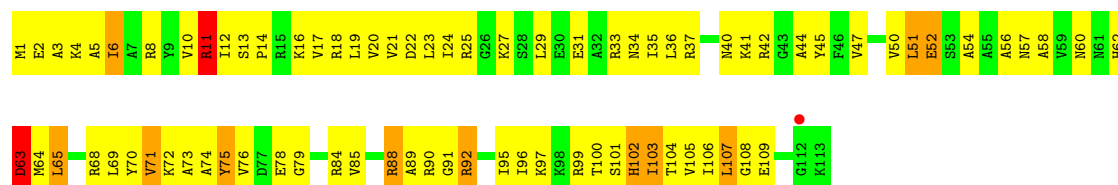
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



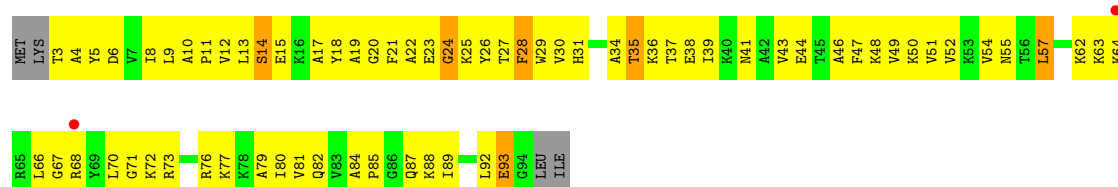
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



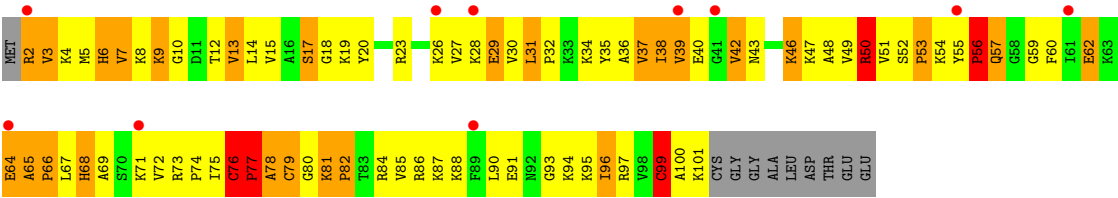
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



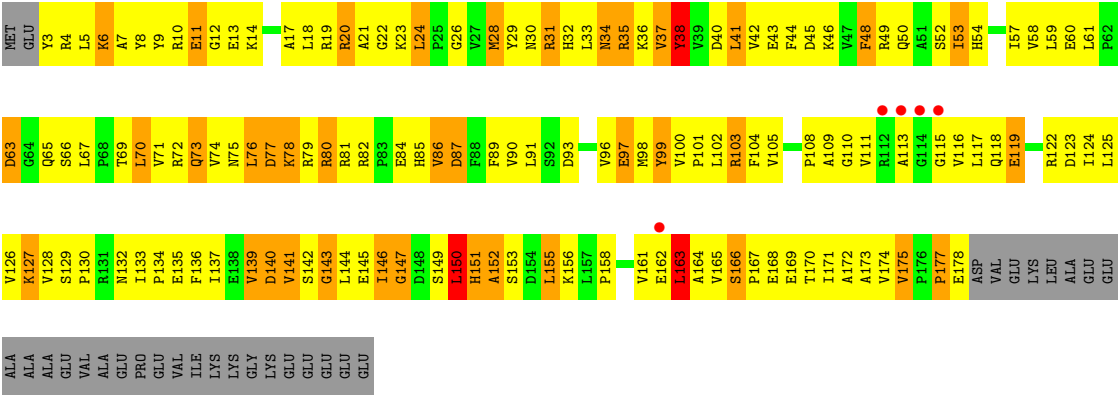
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	197.60Å 274.93Å 282.46Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 48.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-3.10) 95.9 (48.00-3.01)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.231 , 0.268 0.237 , 0.272	Depositor DCC
R_{free} test set	28503 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.6	EDS
Estimated twinning fraction	0.018 for -h,l,k 0.019 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 569519 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	153628	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, PAR, 4SU, GCP, MIA, MG, H2U, ZN, 7MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.58	3/36190 (0.0%)	0.77	49/56486 (0.1%)
2	AB	0.44	0/1935	0.72	1/2609 (0.0%)
3	AC	0.50	1/1636 (0.1%)	0.75	0/2205
4	AD	0.44	0/1733	0.71	1/2318 (0.0%)
5	AE	0.54	0/1162	0.75	0/1564
6	AF	0.45	0/856	0.69	1/1154 (0.1%)
7	AG	0.43	0/1276	0.66	0/1709
8	AH	0.45	0/1136	0.73	0/1527
9	AI	0.45	0/1029	0.71	0/1378
10	AJ	0.49	0/807	0.78	0/1085
11	AK	0.45	0/900	0.72	0/1213
12	AL	0.58	0/986	0.88	2/1320 (0.2%)
13	AM	0.42	0/998	0.79	2/1336 (0.1%)
14	AN	0.54	0/501	0.79	0/664
15	AO	0.42	0/745	0.66	0/992
16	AP	0.44	0/716	0.74	0/963
17	AQ	0.44	0/836	0.70	0/1117
18	AR	0.47	0/579	0.76	0/768
19	AS	0.44	0/642	0.72	0/865
20	AT	0.39	0/765	0.72	1/1007 (0.1%)
21	AU	0.45	0/212	0.69	0/277
22	AV	0.49	0/1809	0.75	0/2819
22	AW	0.45	0/1809	0.73	0/2819
23	AX	0.65	0/334	0.81	0/519
24	AY	0.49	1/1618 (0.1%)	0.78	3/2514 (0.1%)
25	AZ	0.41	0/3203	0.68	1/4346 (0.0%)
26	B0	0.39	0/671	0.73	0/892
27	B1	0.44	0/738	0.74	0/981
28	B2	0.35	0/600	0.63	0/793
29	B3	0.37	0/472	0.66	0/634
30	B4	0.41	0/349	0.60	0/474
31	B5	0.38	0/473	0.72	0/639

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B6	0.66	0/440	0.98	2/586 (0.3%)
33	B7	0.43	0/426	0.71	0/561
34	B8	0.55	0/515	0.83	1/679 (0.1%)
35	B9	0.45	0/310	0.65	0/407
36	BA	0.51	2/69976 (0.0%)	0.74	57/109244 (0.1%)
37	BB	0.40	0/2853	0.72	0/4451
38	BC	0.42	2/1774 (0.1%)	0.67	0/2391
39	BD	0.57	0/2195	0.91	3/2955 (0.1%)
40	BE	0.41	0/1596	0.71	0/2153
41	BF	0.37	0/1658	0.68	0/2244
42	BG	0.37	0/1499	0.68	1/2016 (0.0%)
43	BH	0.36	0/1245	0.70	0/1682
46	BN	0.36	0/1131	0.69	0/1525
47	BO	0.50	0/943	0.76	0/1269
48	BP	0.48	0/1131	0.98	4/1504 (0.3%)
49	BQ	0.45	0/1143	0.69	0/1527
50	BR	0.35	0/974	0.74	1/1302 (0.1%)
51	BS	0.42	0/778	0.77	0/1036
52	BT	0.44	0/1155	0.80	2/1542 (0.1%)
53	BU	0.39	0/975	0.65	0/1297
54	BV	0.36	0/790	0.70	0/1057
55	BW	0.37	0/907	0.68	0/1216
56	BX	0.43	0/739	0.66	1/993 (0.1%)
57	BY	0.38	0/788	0.73	0/1051
58	BZ	0.39	0/1435	0.67	0/1949
All	All	0.50	9/165092 (0.0%)	0.74	133/246624 (0.1%)

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	3	51
23	AX	0	1
24	AY	2	1
36	BA	4	70
37	BB	0	2
All	All	9	125

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	761	A	C5-C6	-8.40	1.33	1.41
24	AY	1	A	OP3-P	-6.72	1.53	1.61
38	BC	120	MET	CG-SD	6.37	1.97	1.81
1	AA	1267	C	C5'-C4'	6.34	1.58	1.51
36	BA	2506	U	N1-C2	5.99	1.44	1.38

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1498	U	C2'-C3'-O3'	10.24	132.03	109.50
1	AA	508	C	C2'-C3'-O3'	10.16	131.85	109.50
36	BA	654(I)	C	N1-C1'-C2'	10.03	127.04	114.00
24	AY	75	C	C2'-C3'-O3'	9.40	130.19	109.50
36	BA	1799	G	C2'-C3'-O3'	9.36	130.09	109.50

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
1	AA	1498	U	C3'
1	AA	1504	G	C3'
24	AY	36	A	C3'
24	AY	75	C	C3'

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	198	G	Sidechain
1	AA	250	A	Sidechain
1	AA	50	A	Sidechain
1	AA	62	U	Sidechain
1	AA	7	G	Sidechain

5.2 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1085	2
2	AB	1900	0	1951	250	0
3	AC	1612	0	1677	139	0
4	AD	1703	0	1764	151	0
5	AE	1146	0	1207	100	0
6	AF	843	0	857	52	0
7	AG	1257	0	1296	120	0
8	AH	1116	0	1177	91	0
9	AI	1011	0	1043	128	0
10	AJ	794	0	840	135	0
11	AK	885	0	904	76	0
12	AL	970	0	1057	110	0
13	AM	987	0	1059	131	0
14	AN	492	0	529	66	0
15	AO	734	0	771	61	0
16	AP	700	0	720	65	0
17	AQ	823	0	891	82	0
18	AR	574	0	644	37	0
19	AS	629	0	652	125	0
20	AT	763	0	861	107	0
21	AU	208	0	221	29	0
22	AV	1619	0	822	61	0
22	AW	1619	0	822	86	0
23	AX	298	0	152	26	0
24	AY	1644	0	853	68	0
25	AZ	3142	0	3152	385	0
26	B0	662	0	688	107	0
27	B1	731	0	808	83	0
28	B2	598	0	653	77	0
29	B3	467	0	523	59	0
30	B4	340	0	337	57	0
31	B5	459	0	480	79	0
32	B6	433	0	461	135	0
33	B7	418	0	467	31	0
34	B8	507	0	576	104	0
35	B9	307	0	335	48	0
36	BA	62477	0	31497	2445	2
37	BB	2551	0	1295	115	0
38	BC	1742	0	1800	349	0
39	BD	2145	0	2234	324	0
40	BE	1563	0	1629	273	0
41	BF	1623	0	1677	250	0
42	BG	1474	0	1535	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BH	1222	0	1282	170	0
44	BJ	651	0	152	15	0
45	BK	700	0	166	13	0
46	BN	1104	0	1180	181	0
47	BO	933	0	996	92	0
48	BP	1114	0	1187	297	0
49	BQ	1122	0	1179	149	0
50	BR	960	0	1021	148	0
51	BS	770	0	832	169	0
52	BT	1141	0	1202	250	0
53	BU	958	0	1015	159	0
54	BV	779	0	852	127	0
55	BW	896	0	953	104	0
56	BX	725	0	778	97	0
57	BY	775	0	870	197	0
58	BZ	1403	0	1432	241	0
59	AA	42	0	45	2	0
60	AD	1	0	0	1	0
60	AN	1	0	0	0	0
60	B4	1	0	0	0	0
60	B9	1	0	0	0	0
61	AZ	32	0	14	5	0
62	AZ	1	0	0	0	0
63	AZ	1	0	0	0	0
All	All	153628	0	104391	9952	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

The worst 5 of 9952 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
36:BA:1899:G:N2	36:BA:1902:C:H41	1.36	1.21
36:BA:2833:G:H3'	36:BA:2834:G:H5''	1.24	1.20
24:AY:1:A:H5'	25:AZ:90:LYS:HZ2	1.06	1.17
55:BW:14:PRO:HG2	55:BW:78:GLU:HG3	1.22	1.17
2:AB:84:GLU:HB3	2:AB:219:VAL:HG21	1.22	1.17

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:1267:C:O5'	36:BA:654(I):C:O4'[2_746]	1.83	0.37

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:1266:G:O3'	36:BA:654(I):C:O4'[2_746]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/256 (91%)	163 (70%)	41 (18%)	28 (12%)	1	4
3	AC	204/239 (85%)	155 (76%)	33 (16%)	16 (8%)	1	11
4	AD	206/209 (99%)	157 (76%)	34 (16%)	15 (7%)	2	12
5	AE	148/162 (91%)	125 (84%)	16 (11%)	7 (5%)	4	23
6	AF	99/101 (98%)	81 (82%)	11 (11%)	7 (7%)	2	12
7	AG	153/156 (98%)	118 (77%)	25 (16%)	10 (6%)	2	15
8	AH	136/138 (99%)	118 (87%)	16 (12%)	2 (2%)	15	57
9	AI	125/128 (98%)	83 (66%)	29 (23%)	13 (10%)	1	5
10	AJ	96/105 (91%)	67 (70%)	17 (18%)	12 (12%)	1	3
11	AK	117/129 (91%)	94 (80%)	19 (16%)	4 (3%)	6	32
12	AL	122/135 (90%)	89 (73%)	20 (16%)	13 (11%)	1	5
13	AM	122/126 (97%)	74 (61%)	27 (22%)	21 (17%)	0	0
14	AN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	0
15	AO	86/89 (97%)	65 (76%)	17 (20%)	4 (5%)	4	23
16	AP	81/88 (92%)	62 (76%)	14 (17%)	5 (6%)	2	16
17	AQ	97/105 (92%)	74 (76%)	18 (19%)	5 (5%)	3	21
18	AR	68/88 (77%)	49 (72%)	14 (21%)	5 (7%)	2	11
19	AS	76/93 (82%)	41 (54%)	21 (28%)	14 (18%)	0	0
20	AT	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	1	10
21	AU	22/27 (82%)	17 (77%)	4 (18%)	1 (4%)	4	24
25	AZ	403/405 (100%)	285 (71%)	83 (21%)	35 (9%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B0	82/85 (96%)	65 (79%)	12 (15%)	5 (6%)	2	16
27	B1	91/98 (93%)	73 (80%)	9 (10%)	9 (10%)	1	6
28	B2	69/72 (96%)	46 (67%)	15 (22%)	8 (12%)	1	4
29	B3	57/60 (95%)	40 (70%)	9 (16%)	8 (14%)	0	2
30	B4	42/71 (59%)	23 (55%)	11 (26%)	8 (19%)	0	0
31	B5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	1	3
32	B6	48/54 (89%)	23 (48%)	12 (25%)	13 (27%)	0	0
33	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
34	B8	61/65 (94%)	34 (56%)	17 (28%)	10 (16%)	0	0
35	B9	35/37 (95%)	21 (60%)	9 (26%)	5 (14%)	0	2
38	BC	226/229 (99%)	161 (71%)	46 (20%)	19 (8%)	1	9
39	BD	273/276 (99%)	219 (80%)	28 (10%)	26 (10%)	1	7
40	BE	202/206 (98%)	116 (57%)	53 (26%)	33 (16%)	0	0
41	BF	205/210 (98%)	144 (70%)	35 (17%)	26 (13%)	0	3
42	BG	179/182 (98%)	107 (60%)	47 (26%)	25 (14%)	0	2
43	BH	157/180 (87%)	96 (61%)	42 (27%)	19 (12%)	1	4
46	BN	136/140 (97%)	93 (68%)	21 (15%)	22 (16%)	0	0
47	BO	120/122 (98%)	97 (81%)	16 (13%)	7 (6%)	3	18
48	BP	144/150 (96%)	74 (51%)	36 (25%)	34 (24%)	0	0
49	BQ	139/141 (99%)	108 (78%)	24 (17%)	7 (5%)	3	22
50	BR	115/118 (98%)	72 (63%)	28 (24%)	15 (13%)	0	3
51	BS	96/112 (86%)	37 (38%)	37 (38%)	22 (23%)	0	0
52	BT	135/146 (92%)	85 (63%)	27 (20%)	23 (17%)	0	0
53	BU	115/118 (98%)	72 (63%)	34 (30%)	9 (8%)	1	11
54	BV	99/101 (98%)	69 (70%)	13 (13%)	17 (17%)	0	0
55	BW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	10
56	BX	90/96 (94%)	67 (74%)	15 (17%)	8 (9%)	1	8
57	BY	98/110 (89%)	45 (46%)	26 (26%)	27 (28%)	0	0
58	BZ	174/206 (84%)	108 (62%)	39 (22%)	27 (16%)	0	1
All	All	6150/6553 (94%)	4274 (70%)	1193 (19%)	683 (11%)	1	5

5 of 683 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	191	ASP
2	AB	194	PRO
2	AB	195	ASP
3	AC	146	ALA
4	AD	4	TYR

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%)	171 (85%)	31 (15%)	4	15
3	AC	160/188 (85%)	139 (87%)	21 (13%)	6	23
4	AD	180/181 (99%)	159 (88%)	21 (12%)	8	29
5	AE	115/123 (94%)	96 (84%)	19 (16%)	3	12
6	AF	90/90 (100%)	79 (88%)	11 (12%)	7	26
7	AG	126/127 (99%)	118 (94%)	8 (6%)	25	66
8	AH	119/119 (100%)	104 (87%)	15 (13%)	7	24
9	AI	98/99 (99%)	85 (87%)	13 (13%)	6	22
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	4	17
11	AK	90/99 (91%)	80 (89%)	10 (11%)	9	33
12	AL	104/111 (94%)	88 (85%)	16 (15%)	4	15
13	AM	99/101 (98%)	85 (86%)	14 (14%)	5	20
14	AN	49/50 (98%)	39 (80%)	10 (20%)	2	8
15	AO	79/80 (99%)	73 (92%)	6 (8%)	19	58
16	AP	72/74 (97%)	64 (89%)	8 (11%)	9	33
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	20	59
18	AR	61/77 (79%)	55 (90%)	6 (10%)	12	40
19	AS	69/80 (86%)	54 (78%)	15 (22%)	1	6
20	AT	76/82 (93%)	66 (87%)	10 (13%)	6	23
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	72
25	AZ	339/339 (100%)	289 (85%)	50 (15%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	B0	66/67 (98%)	55 (83%)	11 (17%)	3	11
27	B1	78/83 (94%)	65 (83%)	13 (17%)	3	11
28	B2	66/67 (98%)	61 (92%)	5 (8%)	19	58
29	B3	51/52 (98%)	48 (94%)	3 (6%)	28	68
30	B4	39/63 (62%)	30 (77%)	9 (23%)	1	5
31	B5	51/52 (98%)	46 (90%)	5 (10%)	12	40
32	B6	49/52 (94%)	39 (80%)	10 (20%)	2	8
33	B7	41/42 (98%)	35 (85%)	6 (15%)	5	18
34	B8	53/55 (96%)	43 (81%)	10 (19%)	2	9
35	B9	34/34 (100%)	27 (79%)	7 (21%)	2	8
38	BC	180/181 (99%)	159 (88%)	21 (12%)	8	29
39	BD	217/218 (100%)	175 (81%)	42 (19%)	2	8
40	BE	165/166 (99%)	142 (86%)	23 (14%)	5	21
41	BF	165/166 (99%)	149 (90%)	16 (10%)	12	41
42	BG	155/156 (99%)	132 (85%)	23 (15%)	4	17
43	BH	132/148 (89%)	124 (94%)	8 (6%)	26	67
46	BN	117/119 (98%)	102 (87%)	15 (13%)	6	24
47	BO	100/100 (100%)	92 (92%)	8 (8%)	17	55
48	BP	112/116 (97%)	87 (78%)	25 (22%)	1	6
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	7	24
50	BR	100/101 (99%)	81 (81%)	19 (19%)	2	9
51	BS	77/88 (88%)	66 (86%)	11 (14%)	5	19
52	BT	120/127 (94%)	96 (80%)	24 (20%)	2	8
53	BU	92/94 (98%)	81 (88%)	11 (12%)	7	27
54	BV	82/82 (100%)	72 (88%)	10 (12%)	7	26
55	BW	91/92 (99%)	80 (88%)	11 (12%)	7	27
56	BX	74/78 (95%)	68 (92%)	6 (8%)	17	53
57	BY	84/91 (92%)	71 (84%)	13 (16%)	4	14
58	BZ	155/179 (87%)	129 (83%)	26 (17%)	3	11
All	All	5186/5431 (96%)	4476 (86%)	710 (14%)	5	21

5 of 710 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	B1	43	TYR
38	BC	147	PHE
55	BW	52	GLU
28	B2	7	ARG
32	B6	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
26	B0	50	ASN
34	B8	35	GLN
55	BW	57	ASN
27	B1	45	ASN
29	B3	52	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	247 (16%)	56 (3%)
22	AV	75/76 (98%)	22 (29%)	0
22	AW	75/76 (98%)	17 (22%)	0
23	AX	13/14 (92%)	2 (15%)	1 (7%)
24	AY	74/77 (96%)	23 (31%)	2 (2%)
36	BA	2900/2915 (99%)	547 (18%)	52 (1%)
37	BB	118/122 (96%)	24 (20%)	2 (1%)
All	All	4758/4802 (99%)	882 (18%)	113 (2%)

5 of 882 RNA backbone outliers are listed below:

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

5 of 113 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1319	A
36	BA	221	A

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Mol	Chain	Res	Type
36	BA	2439	A
1	AA	1399	C
24	AY	18	G

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	H2U	AY	16	24	19,21,22	0.99	0	27,30,33	1.79	5 (18%)
24	H2U	AY	17	24	19,21,22	1.09	2 (10%)	27,30,33	1.80	5 (18%)
24	H2U	AY	20	24	19,21,22	1.04	0	27,30,33	1.93	7 (25%)
24	OMC	AY	32	24	20,22,23	1.19	3 (15%)	25,31,34	0.89	2 (8%)
24	MIA	AY	37	24	29,31,32	1.03	2 (6%)	41,44,47	1.59	6 (14%)
24	7MG	AY	46	24	24,26,27	2.33	4 (16%)	34,39,42	2.35	6 (17%)
24	5MU	AY	54	24	20,22,23	1.17	3 (15%)	25,32,35	1.59	3 (12%)
24	PSU	AY	55	24	19,21,22	1.01	1 (5%)	23,30,33	1.19	4 (17%)
24	4SU	AY	8	24	19,21,22	1.31	2 (10%)	23,30,33	23.88	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	16	24	-	0/8/38/39	0/2/2/2
24	H2U	AY	17	24	-	0/8/38/39	0/2/2/2
24	H2U	AY	20	24	-	0/8/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/8/27/28	0/2/2/2
24	MIA	AY	37	24	-	0/16/33/34	0/3/3/3
24	7MG	AY	46	24	-	0/8/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5MU	AY	54	24	-	0/6/25/26	0/2/2/2
24	PSU	AY	55	24	-	0/8/25/26	0/2/2/2
24	4SU	AY	8	24	-	0/6/25/26	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-10.07	1.38	1.46
24	AY	8	4SU	C5-C4	3.36	1.42	1.38
24	AY	32	OMC	C2-N1	2.97	1.41	1.38
24	AY	46	7MG	C8-N7	-2.92	1.30	1.44
24	AY	55	PSU	C6-N1	2.87	1.40	1.35

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	8	4SU	C4-N3-C2	114.48	126.50	121.60
24	AY	46	7MG	C6-N1-C2	8.78	125.16	120.20
24	AY	46	7MG	N7-C8-N9	7.61	113.23	103.13
24	AY	54	5MU	C6-N1-C2	-6.24	120.63	122.41
24	AY	37	MIA	C11-S10-C2	5.10	105.94	102.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	PAR	AA	1601	-	45,45,45	1.43	5 (11%)	67,67,67	1.25	5 (7%)
61	GCP	AZ	501	62	34,34,34	2.65	11 (32%)	52,54,54	3.31	15 (28%)

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	PAR	AA	1601	-	-	0/18/94/94	0/4/4/4
61	GCP	AZ	501	62	-	0/20/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	501	GCP	PG-C3B	8.92	1.88	1.79
61	AZ	501	GCP	C6-N1	5.78	1.45	1.36
61	AZ	501	GCP	C5-N7	-5.39	1.31	1.38
61	AZ	501	GCP	PG-O2G	-4.50	1.45	1.54
61	AZ	501	GCP	PB-C3B	4.06	1.83	1.79

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AZ	501	GCP	C6-C5-N7	-20.43	131.39	134.14
59	AA	1601	PAR	O33-C14-C24	4.23	116.45	108.08
61	AZ	501	GCP	N1-C2-N3	4.16	127.40	121.78
61	AZ	501	GCP	C2-N3-C4	-4.00	110.50	115.30
59	AA	1601	PAR	O54-C54-C64	3.81	113.23	105.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.06	32 (2%) 60 11	25, 58, 149, 200	0
2	AB	234/256 (91%)	-0.04	1 (0%) 90 45	35, 74, 133, 147	0
3	AC	206/239 (86%)	-0.25	0 100 100	34, 57, 91, 103	0
4	AD	208/209 (99%)	-0.10	0 100 100	44, 68, 96, 102	0
5	AE	150/162 (92%)	-0.27	0 100 100	33, 52, 82, 102	0
6	AF	101/101 (100%)	-0.12	1 (0%) 79 23	52, 74, 89, 100	0
7	AG	155/156 (99%)	-0.19	0 100 100	46, 71, 96, 119	0
8	AH	138/138 (100%)	-0.20	0 100 100	38, 58, 78, 87	0
9	AI	127/128 (99%)	-0.00	2 (1%) 68 15	41, 74, 103, 112	0
10	AJ	98/105 (93%)	0.02	1 (1%) 79 23	35, 75, 111, 117	0
11	AK	119/129 (92%)	-0.10	1 (0%) 83 28	39, 59, 95, 117	0
12	AL	124/135 (91%)	-0.12	2 (1%) 68 15	36, 48, 77, 112	0
13	AM	124/126 (98%)	0.16	6 (4%) 29 4	50, 80, 107, 132	0
14	AN	60/61 (98%)	-0.19	0 100 100	32, 48, 76, 83	0
15	AO	88/89 (98%)	-0.08	0 100 100	42, 64, 89, 93	0
16	AP	83/88 (94%)	-0.07	0 100 100	50, 65, 85, 114	0
17	AQ	99/105 (94%)	-0.05	0 100 100	45, 70, 95, 97	0
18	AR	70/88 (79%)	-0.08	0 100 100	46, 65, 97, 111	0
19	AS	78/93 (83%)	0.24	1 (1%) 74 19	58, 84, 115, 123	0
20	AT	99/106 (93%)	0.26	1 (1%) 79 23	56, 86, 128, 131	0
21	AU	24/27 (88%)	0.01	0 100 100	52, 64, 79, 91	0
22	AV	76/76 (100%)	0.83	10 (13%) 4 1	35, 127, 168, 176	0
22	AW	76/76 (100%)	1.90	34 (44%) 1 0	60, 175, 200, 200	0
23	AX	14/14 (100%)	0.69	2 (14%) 3 1	35, 57, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
24	AY	76/77 (98%)	0.40	2 (2%) 53 8	47, 110, 183, 198	0
25	AZ	405/405 (100%)	0.08	1 (0%) 93 61	57, 100, 135, 143	0
26	B0	84/85 (98%)	0.33	6 (7%) 16 3	59, 75, 116, 136	0
27	B1	93/98 (94%)	0.03	0 100 100	44, 65, 106, 114	0
28	B2	71/72 (98%)	0.33	2 (2%) 50 8	75, 108, 124, 146	0
29	B3	59/60 (98%)	0.41	2 (3%) 43 6	72, 93, 110, 135	0
30	B4	44/71 (61%)	0.27	0 100 100	103, 134, 142, 149	0
31	B5	59/60 (98%)	0.33	4 (6%) 17 3	57, 89, 151, 155	0
32	B6	50/54 (92%)	0.41	1 (2%) 62 12	52, 81, 99, 108	0
33	B7	48/49 (97%)	0.04	0 100 100	49, 59, 99, 117	0
34	B8	63/65 (96%)	0.15	0 100 100	53, 73, 91, 106	0
35	B9	37/37 (100%)	0.50	2 (5%) 25 4	61, 82, 96, 97	0
36	BA	2901/2915 (99%)	0.24	194 (6%) 17 3	28, 76, 190, 200	0
37	BB	119/122 (97%)	0.06	3 (2%) 54 9	74, 103, 134, 150	0
38	BC	228/229 (99%)	1.82	81 (35%) 1 0	125, 160, 177, 186	0
39	BD	275/276 (99%)	-0.19	1 (0%) 90 45	24, 45, 71, 93	0
40	BE	204/206 (99%)	0.14	3 (1%) 70 16	50, 77, 128, 135	0
41	BF	207/210 (98%)	0.35	7 (3%) 43 6	47, 97, 149, 155	0
42	BG	181/182 (99%)	0.18	3 (1%) 67 15	79, 101, 126, 137	0
43	BH	159/180 (88%)	0.43	7 (4%) 33 5	80, 119, 144, 150	0
44	BJ	0/130	-	-	-	-
45	BK	0/140	-	-	-	-
46	BN	138/140 (98%)	0.19	3 (2%) 59 11	68, 93, 127, 132	0
47	BO	122/122 (100%)	-0.21	0 100 100	42, 59, 72, 83	0
48	BP	146/150 (97%)	0.35	3 (2%) 60 11	55, 90, 121, 146	0
49	BQ	141/141 (100%)	-0.00	2 (1%) 72 17	50, 68, 100, 134	0
50	BR	117/118 (99%)	0.11	1 (0%) 81 25	58, 81, 100, 105	0
51	BS	98/112 (87%)	0.24	3 (3%) 47 7	70, 93, 121, 126	0
52	BT	137/146 (93%)	0.15	5 (3%) 41 6	54, 80, 139, 161	0
53	BU	117/118 (99%)	0.13	2 (1%) 67 15	68, 88, 113, 120	0
54	BV	101/101 (100%)	0.50	2 (1%) 62 12	67, 117, 132, 137	0
55	BW	113/113 (100%)	0.12	1 (0%) 81 25	65, 88, 115, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BX	92/96 (95%)	0.29	2 (2%) 59 11	65, 85, 101, 107	0
57	BY	100/110 (90%)	0.93	10 (10%) 8 2	94, 125, 149, 158	0
58	BZ	176/206 (85%)	0.32	5 (2%) 50 8	69, 102, 125, 134	0
All	All	11016/11625 (94%)	0.16	452 (4%) 35 5	24, 77, 158, 200	0

The worst 5 of 452 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BA	1073	A	10.3
36	BA	654(P)	C	9.6
36	BA	1075	C	8.8
36	BA	271(N)	U	8.6
36	BA	1074	G	8.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	PSU	AY	55	20/21	0.28	-	154,158,159,160	0
24	H2U	AY	17	20/21	0.79	-	191,199,200,200	0
24	MIA	AY	37	29/30	0.27	-	48,63,74,86	0
24	OMC	AY	32	21/22	0.23	-	76,80,87,88	0
24	5MU	AY	54	21/22	0.33	-	145,152,154,155	0
24	H2U	AY	20	20/21	0.37	-	185,187,191,191	0
24	7MG	AY	46	24/25	0.28	-	112,114,120,121	0
24	H2U	AY	16	20/21	0.44	-	171,185,187,190	0
24	4SU	AY	8	20/21	0.27	-	104,105,107,108	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	ZN	AD	301	1/1	0.32	-	58,58,58,58	0
60	ZN	B9	101	1/1	0.13	-	92,92,92,92	0
60	ZN	B4	101	1/1	0.10	-	132,132,132,132	0
62	MG	AZ	502	1/1	0.23	-	55,55,55,55	0
60	ZN	AN	101	1/1	0.18	-	45,45,45,45	0
59	PAR	AA	1601	42/42	0.22	-	33,42,58,62	0
61	GCP	AZ	501	32/32	0.22	-	89,110,116,117	0

6.5 Other polymers

There are no such residues in this entry.