



# wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 06:35 pm GMT

PDB ID : 8R3V  
EMDB ID : EMD-18875  
Title : Escherichia coli paused disome complex (non-rotated disome interface)  
Authors : Fluegel, T.; Schacherl, M.  
Deposited on : 2023-11-10  
Resolution : 3.28 Å(reported)  
Based on initial model : 7N1P

This is a wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

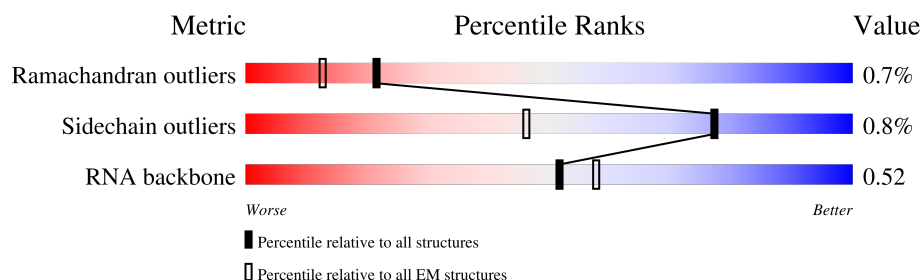
EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.28 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.



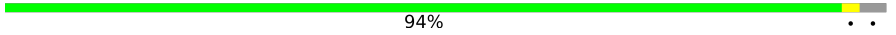



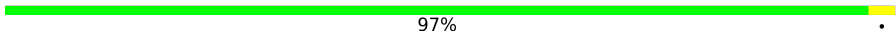
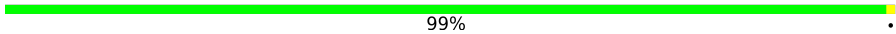
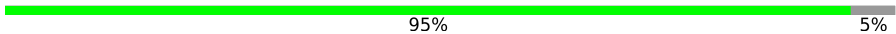
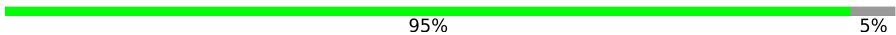






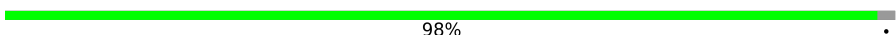
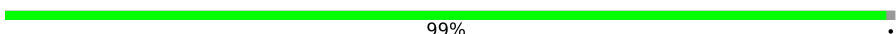
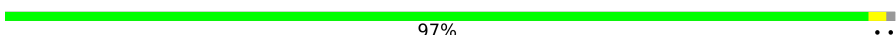



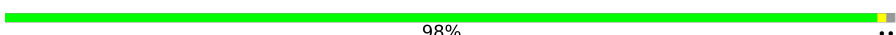
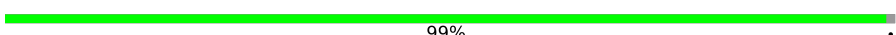
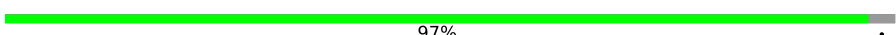
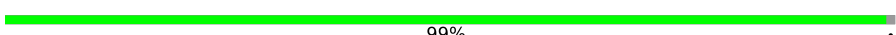
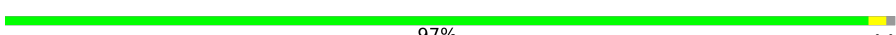
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	12	78	
2	32	59	
3	4	70	
4	62	65	
5	71	2904	
5	72	2904	
6	82	120	
7	A1	1542	
7	A2	1542	

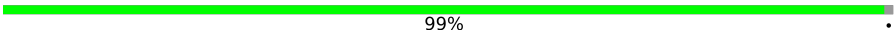
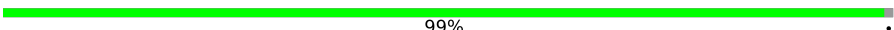
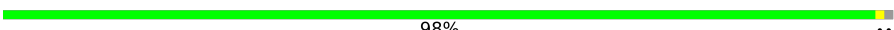
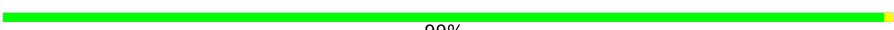
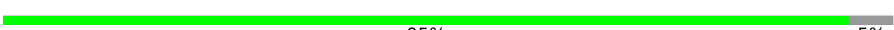





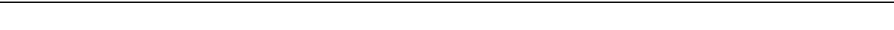

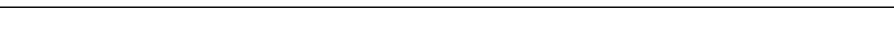
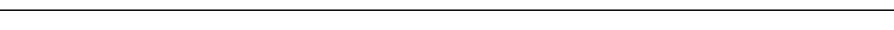






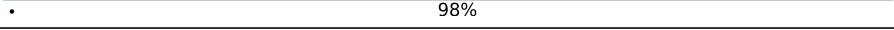

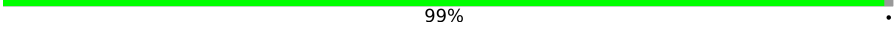
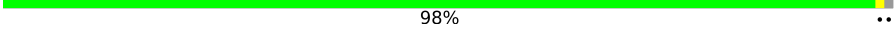
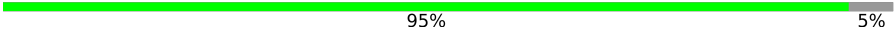
Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
8	B	241	 94% . .
8	B2	241	 92% . 6%
9	C1	233	 90% . 9%
9	C2	233	 91% 9%
10	D1	206	 97% .
10	D2	206	 99% .
11	E1	167	 95% 5%
11	E2	167	 95% 5%
12	F1	135	 79% 21%
12	F2	135	 76% . 21%
13	G1	179	 87% 13%
13	G2	179	 82% . 14%
14	H1	130	 99% .
14	H2	130	 99% .
15	I1	130	 98% .
15	I2	130	 99% .
16	J1	103	 97% . .
16	J2	103	 88% . 9%
17	K1	129	 86% . 11%
17	K2	129	 89% . 9%
18	L1	124	 98% . .
18	L2	124	 99% .
19	M1	118	 97% .
19	M2	118	 99% .
20	N1	101	 97% . .

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
20	N2	101	 99% .
21	O1	89	 99% .
21	O2	89	 98% ..
22	P1	82	 99% .
23	Q1	84	 95% 5%
23	Q2	84	 93% . 5%
24	R1	75	 96% ..
24	R2	75	 93% 5% .
25	S1	92	 89% . 10%
25	S2	92	 90% 10%
26	T1	87	 92% 7% .
27	U1	71	 96% ..
27	U2	71	 96% ..
28	V2	64	 31% 59% 9%
29	W	76	 59% 33% 8%
30	W1	76	 29% 17% . 53%
31	X2	77	 58% 34% 8%
32	Y1	76	 38% 8% . 53%
33	Y2	76	 67% 28% 5%
34	Z1	557	 98% .
35	a2	234	 57% 43%
36	b2	273	 99% .
37	e2	179	 98% ..
38	g2	55	 95% 5%
39	h2	136	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	i2	149	<div><div></div><div>96%</div><div>.</div></div>
41	l2	46	<div><div></div><div>98%</div><div>.</div></div>
42	o2	144	<div><div></div><div>35%</div><div>65%</div></div>
43	p	10	<div><div></div><div>70%</div><div>20%</div><div>10%</div></div>
44	r2	117	<div><div></div><div>99%</div><div>.</div></div>
45	z2	85	<div><div></div><div>89%</div><div>11%</div></div>

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 188607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	12	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	32	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	62	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	71	30	Total	C	N	O	P	0	0
			644	288	119	207	30		
5	72	2904	Total	C	N	O	P	0	0
			62355	27824	11468	20159	2904		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	82	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A1	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		
7	A2	1537	Total	C	N	O	P	0	0
			32990	14721	6049	10683	1537		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	233	Total	C	N	O	S	0	0
			1815	1145	325	337	8		
8	B2	227	Total	C	N	O	S	0	0
			1776	1123	318	327	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	213	Total	C	N	O	S	0	0
			1665	1054	312	295	4		
9	C2	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		
10	D2	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E1	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		
11	E2	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	94	Total	C	N	O	S	0	0
			756	474	147	134	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.



Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	64	Total	C	N	O	P	0	0
			1382	619	267	432	64		

- Molecule 29 is a RNA chain called tRNA-Trp (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	W	76	Total	C	N	O	P	S	0	0
			1630	730	286	536	76	2		

- Molecule 30 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W1	36	Total	C	N	O	P	S	0	0
			781	352	143	248	36	2		

- Molecule 31 is a RNA chain called tRNA-Arg (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	X2	77	Total	C	N	O	P	S	0	0
			1654	740	297	538	77	2		

- Molecule 32 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y1	36	Total	C	N	O	P	0	0
			778	348	142	252	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y1	34	CM0	U	variant	GB 1847302804

- Molecule 33 is a RNA chain called tRNA-Ala (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y2	76	Total	C	N	O	P	0	0
			1628	726	293	533	76		

- Molecule 34 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Z1	9	Total	C	N	O	0	0
			75	49	10	16		

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a2	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 37 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e2	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 38 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	g2	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h2	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i2	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 41 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o2	51	Total	C	N	O	S	0	0
			377	231	83	62	1		

- Molecule 43 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	p	10	Total	C	N	O	0	0
			76	47	18	11		

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r2	116	Total	C	N	O	0	0
			891	552	178	161		

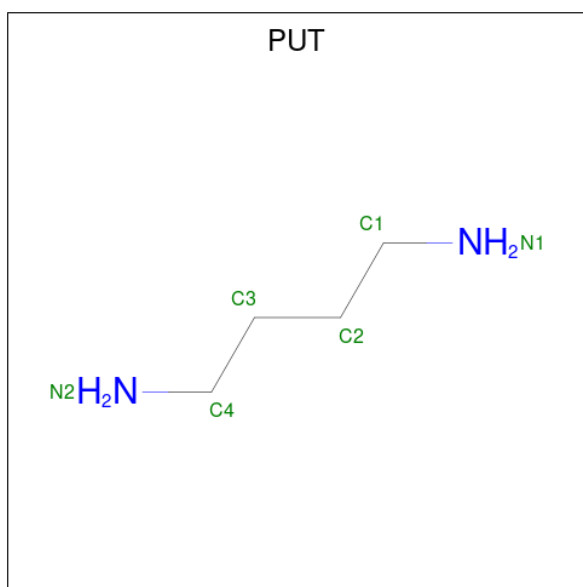
- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z2	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

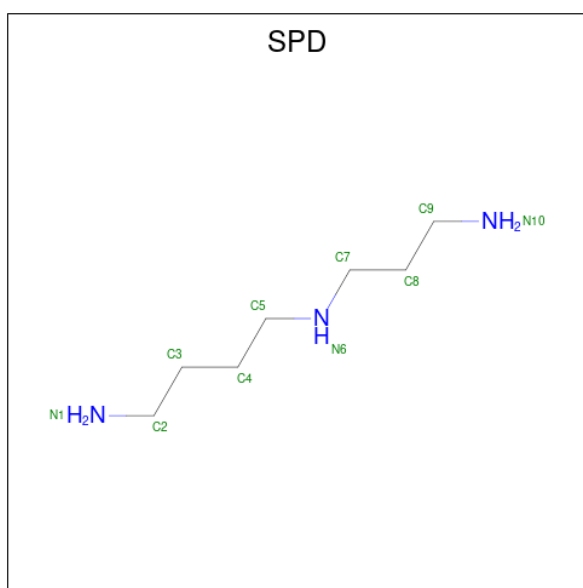
Mol	Chain	Residues	Atoms		AltConf
46	4	1	Total	Zn	0
			1	1	
46	B	1	Total	Zn	0
			1	1	

- Molecule 47 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			6	4	2	
47	72	1	Total	C	N	0
			6	4	2	

- Molecule 48 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).

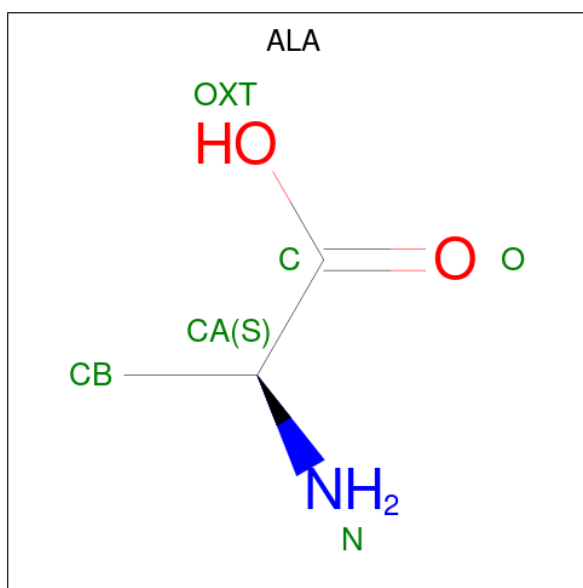


Mol	Chain	Residues	Atoms			AltConf
48	72	1	Total	C	N	0
			10	7	3	

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	72	190	Total	Mg	0
			190	190	
49	82	1	Total	Mg	0
			1	1	
49	A1	60	Total	Mg	0
			60	60	
49	A2	42	Total	Mg	0
			42	42	
49	W	1	Total	Mg	0
			1	1	
49	Y2	1	Total	Mg	0
			1	1	
49	h2	1	Total	Mg	0
			1	1	
49	o2	1	Total	Mg	0
			1	1	

- Molecule 50 is ALANINE (three-letter code: ALA) (formula:  $C_3H_7NO_2$ ).

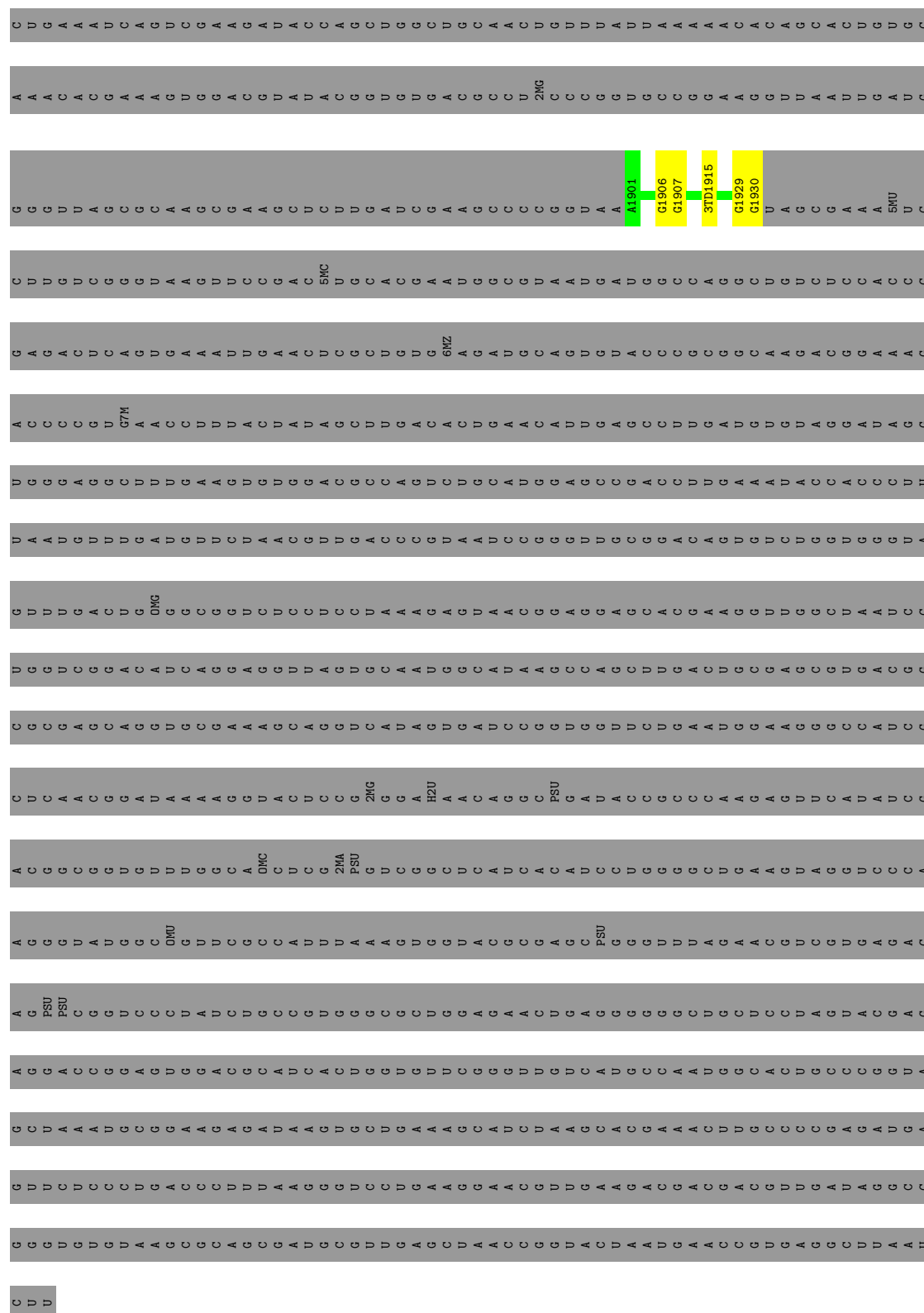


Mol	Chain	Residues	Atoms				AltConf
50	Y2	1	Total	C	N	O	0
			5	3	1	1	

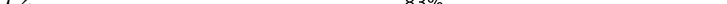


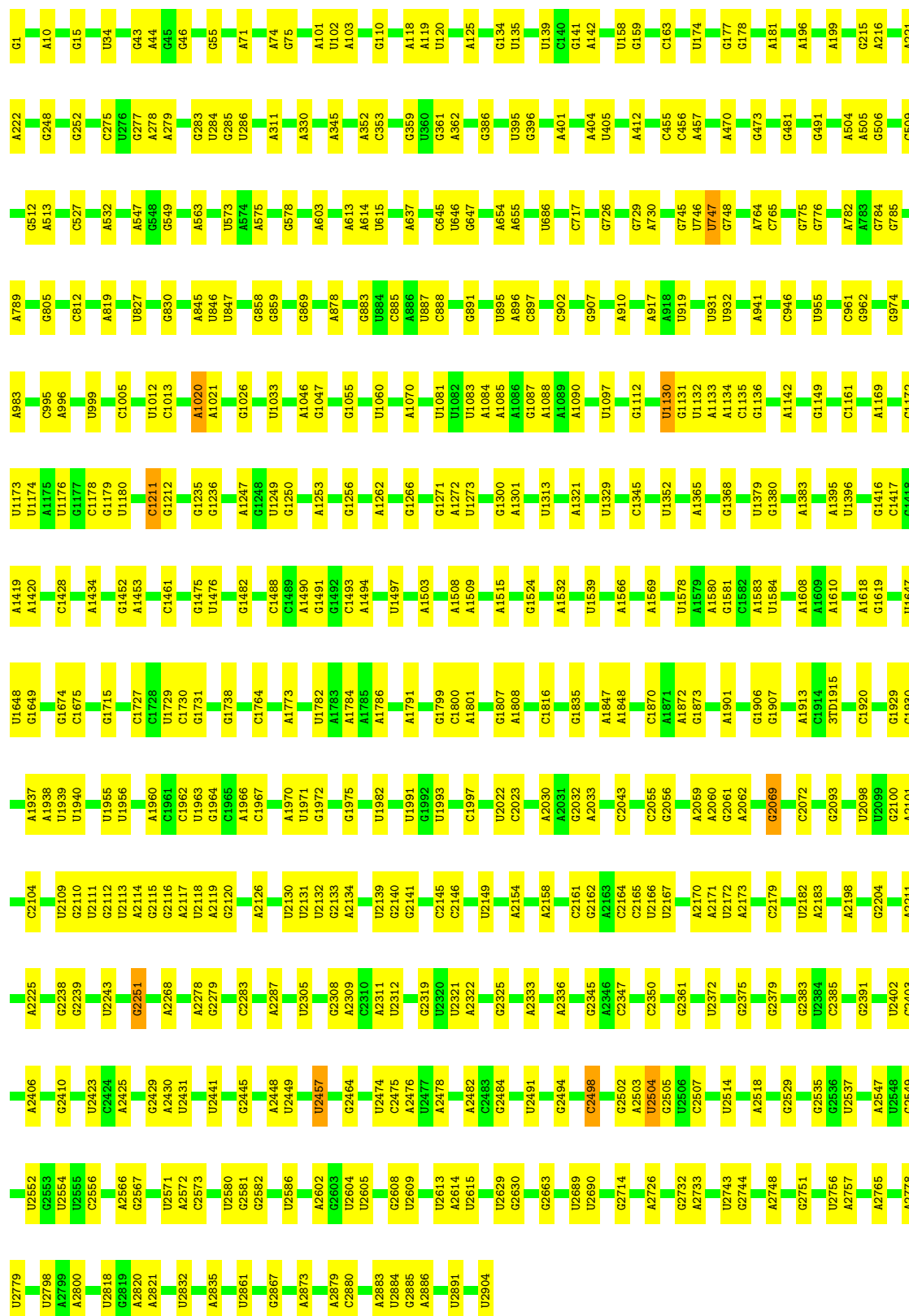


A G U A G C G G C C G A A G C G G A A C G G G A A G C C A G C C C U G A A U C A A G U G G U U A G G G A A  
G C G U C C G G A A A G C G C G C G G A U A C A C A G G G U G A C A G C C C G U A C A A A A A U G C A A C U G G U  
G A G C C U C C A A U G A A G U A A G G C G C G G A A C A C A C G U G G U A U C U G U C U A A U A A G G G G G A C C A C U C  
C A A G G C U A A A A A A C U C C U G A C U A A C A C G A A A A C A A G U A A G G A A A A A A A A A A A A A A A A  
G A A C C C C G G C G A G G G G A  
A C G C C U U A G G C G G U A A C C G G C G G U A A C C C U U U U G U A U A A A A U G G U C A A C G A U U U C U A A G  
C A A G G U U A A A C C G A A U A A G G G A G A A C C G A A A C C G A A A C C U U A A C U U A A C U U A A G U U G C  
A G G G U U A A G A A C C C G A A A A A C C G G U A U C U A A G C C A A U G G C A A G G U U A A G G U U A A C A C U  
A A C U G G A A G A A C C C G A A C U A  
A A A G G C C A A A C C C G G A A C U A  
G U G A A A U U C A A U C C G G G G U A G A  
C C G A U G C A A A C U G C G G A A A C C C G A  
C G U C C G U C G A A A G A G G G A  
A G U G G A A A A C C A A G U G A A G G A  
U U A A A A G A A A A A G C U A  
U A A A C C U G G C A A C G A A A G G A  
U G U A A A G C C U G G A A A G G A  
C A U A A A C G A  
A A C G U U A  
G A  
G G A  
G U U G C C G G G G C A A G G A  
G A  
C U U C C A A G A  
U G G U C A G G A  
G G U G C C G G G G A



- Molecule 5: 23S ribosomal RNA

Chain 72:  83% 17%



• Molecule 6: 5S ribosomal RNA

Chain 82:

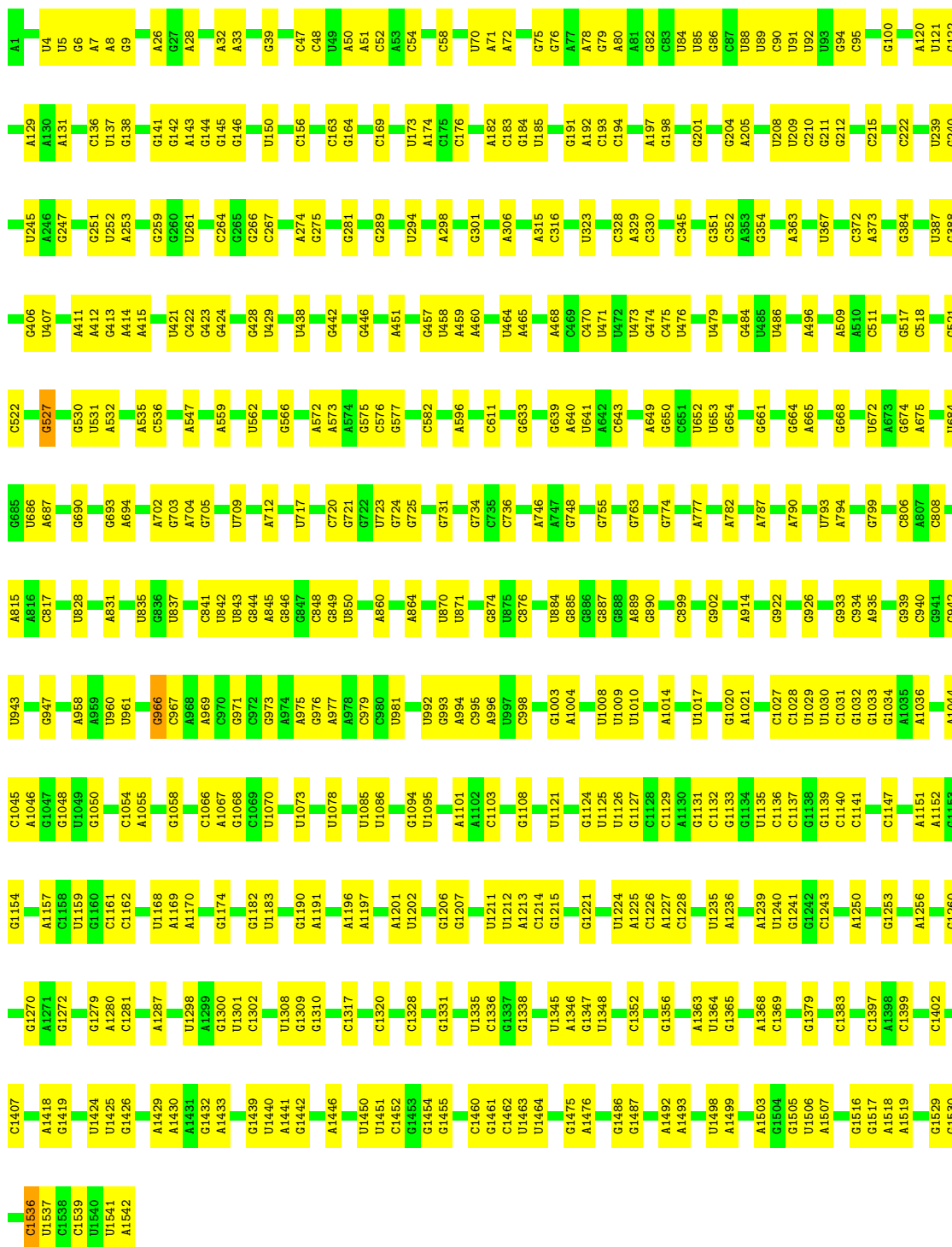
78%

20%



• Molecule 7: 16S ribosomal RNA

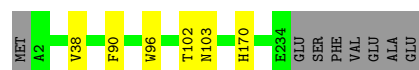
Chain A1: 70% 30%



• Molecule 7: 16S ribosomal RNA

27%

- Molecule 8: Small ribosomal subunit protein uS2



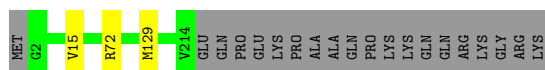
- Molecule 8: Small ribosomal subunit protein uS2

- 6%



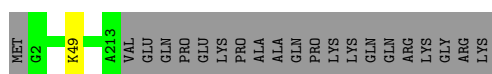
- Molecule 9: Small ribosomal subunit protein uS3

Chain C1: 90% 9%



- Molecule 9: Small ribosomal subunit protein uS3

Chain C2: 91% 9%



- Molecule 10: Small ribosomal subunit protein uS4

Chain D1: 97%



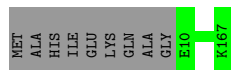
- Molecule 10: Small ribosomal subunit protein uS4

Chain D2: 99%



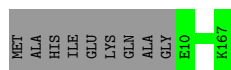
- Molecule 11: Small ribosomal subunit protein uS5

Chain E1: 95% 5%



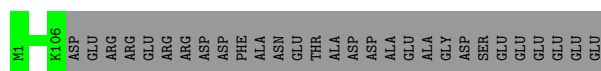
- Molecule 11: Small ribosomal subunit protein uS5

Chain E2: 95% 5%



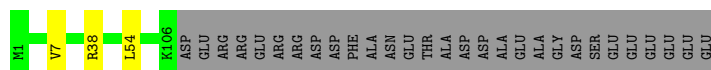
- Molecule 12: 30S ribosomal protein S6

Chain F1: 79% 21%



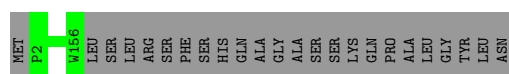
- Molecule 12: 30S ribosomal protein S6

Chain F2: 76% 21%



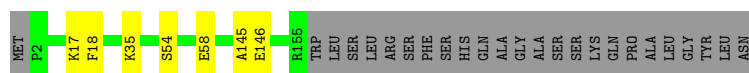
- Molecule 13: 30S ribosomal protein S7

Chain G1: 87% 13%



- Molecule 13: 30S ribosomal protein S7

Chain G2: 82% 14%



- Molecule 14: Small ribosomal subunit protein uS8

Chain H1: 99% .



- Molecule 14: Small ribosomal subunit protein uS8

Chain H2: 99% .



- Molecule 15: Small ribosomal subunit protein uS9

Chain I1: 98% .



- Molecule 15: Small ribosomal subunit protein uS9

Chain I2: 99% .



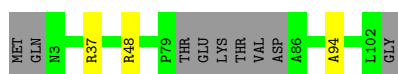
- Molecule 16: 30S ribosomal protein S10

Chain J1: 97%



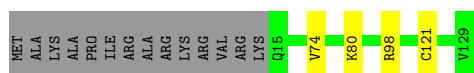
- Molecule 16: 30S ribosomal protein S10

Chain J2: 88%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K1: 86%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K2: 89%



- Molecule 18: Small ribosomal subunit protein uS12

Chain L1: 98%



- Molecule 18: Small ribosomal subunit protein uS12

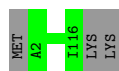
Chain L2: 99%



- Molecule 19: Small ribosomal subunit protein uS13

Chain M1: 97%





- Molecule 19: Small ribosomal subunit protein uS13

Chain M2: 99%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N1: 97%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N2: 99%



- Molecule 21: 30S ribosomal protein S15

Chain O1: 99%



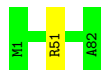
- Molecule 21: 30S ribosomal protein S15

Chain O2: 98%



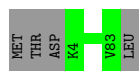
- Molecule 22: 30S ribosomal protein S16

Chain P1: 99%



- Molecule 23: Small ribosomal subunit protein uS17

Chain Q1: 95%



- Molecule 23: Small ribosomal subunit protein uS17

Chain Q2: 93% 5%



- Molecule 24: Small ribosomal subunit protein bS18

Chain R1: 96% 2%



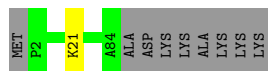
- Molecule 24: Small ribosomal subunit protein bS18

Chain R2: 93% 5%



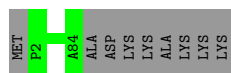
- Molecule 25: Small ribosomal subunit protein uS19

Chain S1: 89% 10%



- Molecule 25: Small ribosomal subunit protein uS19

Chain S2: 90% 10%



- Molecule 26: Small ribosomal subunit protein bS20

Chain T1: 92% 7%



- Molecule 27: 30S ribosomal protein S21

Chain U1: 96% 2%



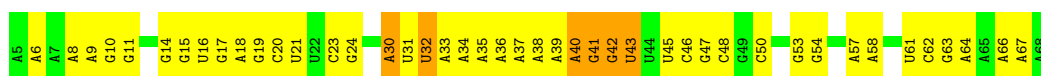
- Molecule 27: 30S ribosomal protein S21

Chain U2: 96%



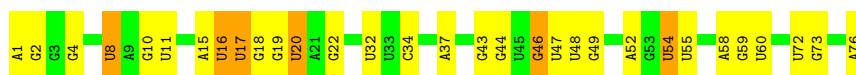
- Molecule 28: messenger RNA

Chain V2: 31% 59% 9%



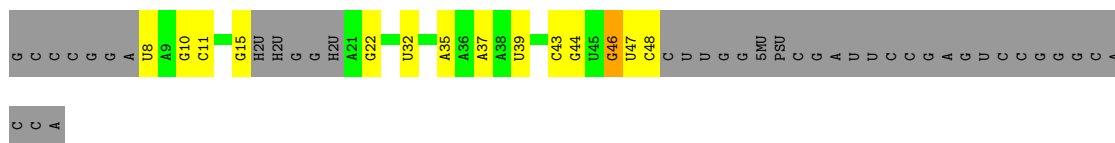
- Molecule 29: tRNA-Trp (P-site)

Chain W: 59% 33% 8%



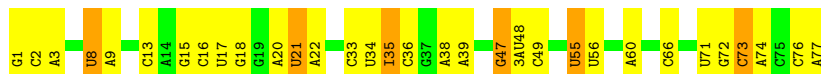
- Molecule 30: tRNA-Phe (P-site)

Chain W1: 29% 17% 53%



- Molecule 31: tRNA-Arg (E-site)

Chain X2: 58% 34% 8%



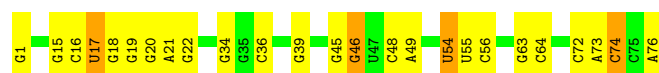
- Molecule 32: tRNA-Val (A-site)

Chain Y1: 38% 8% 53%



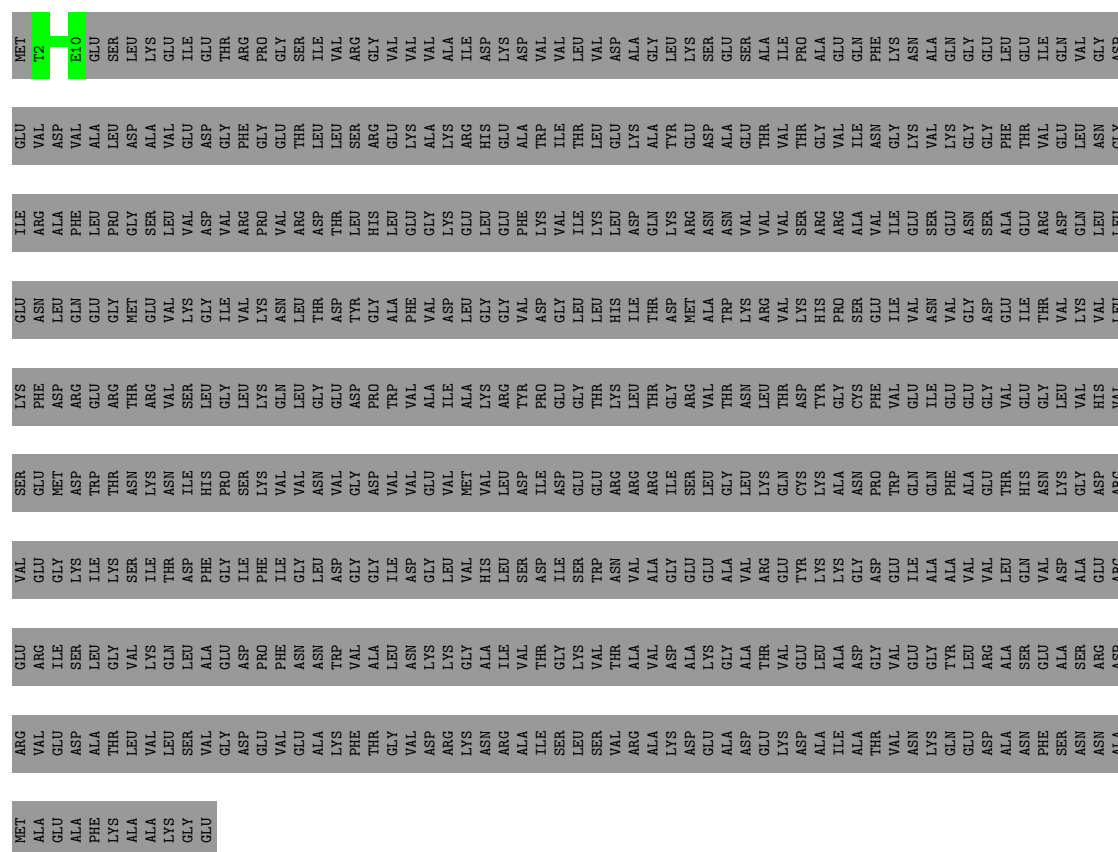
- Molecule 33: tRNA-Ala (A-site)

Chain Y2:  67% 28% 5%



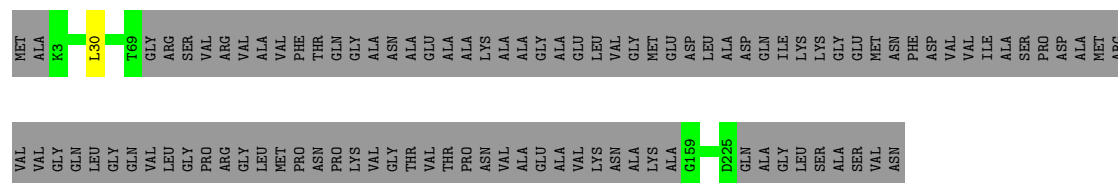
- Molecule 34: 30S ribosomal protein S1

Chain Z1:  98%



- Molecule 35: Large ribosomal subunit protein uL1

Chain a2:  57% 43%



- Molecule 36: 50S ribosomal protein L2

Chain b2:  99%



- Molecule 37: 50S ribosomal protein L5

Chain e2: 98% ..



- Molecule 38: 50S ribosomal protein L33

Chain g2: 95% 5%



- Molecule 39: 50S ribosomal protein L16

Chain h2: 100%

There are no outlier residues recorded for this chain.

- Molecule 40: 50S ribosomal protein L9

Chain i2: 96% .



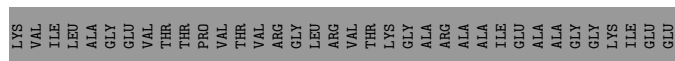
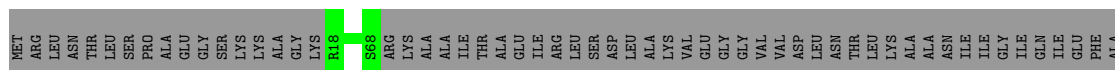
- Molecule 41: 50S ribosomal protein L34

Chain l2: 98% .



- Molecule 42: 50S ribosomal protein L15

Chain o2: 35% 65%



- Molecule 43: Nascent chain

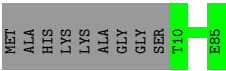
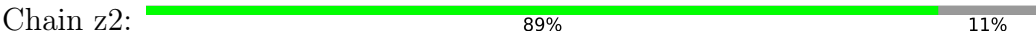
Chain p: 70% 20% 10%



- Molecule 44: 50S ribosomal protein L18



- Molecule 45: 50S ribosomal protein L27



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, H2U, SPD, 3TD, ZN, OMU, PUT, MG, 2MG, 6MZ, 2MA, CM0, PSU, MIA, OMG, 4SU, 7MG, G7M, RSP, 5MC, UR3, 3AU, 1MG, 4OC, OMC, 5MU

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	12	0.24	0/635	0.61	0/848
2	32	0.22	0/453	0.53	0/605
3	4	0.30	0/539	0.73	1/721 (0.1%)
4	62	0.24	0/513	0.57	0/676
5	71	0.15	0/696	0.70	0/1081
5	72	0.17	1/69306 (0.0%)	0.69	9/108116 (0.0%)
6	82	0.21	1/2872 (0.0%)	0.75	3/4478 (0.1%)
7	A1	0.23	0/36794	0.77	1/57392 (0.0%)
7	A2	0.23	0/36681	0.75	7/57217 (0.0%)
8	B	0.25	0/1846	0.54	0/2488
8	B2	0.26	0/1807	0.53	0/2435
9	C1	0.25	0/1692	0.56	0/2280
9	C2	0.26	0/1685	0.56	0/2270
10	D1	0.25	0/1665	0.55	0/2227
10	D2	0.25	0/1665	0.55	0/2227
11	E1	0.26	0/1179	0.52	0/1584
11	E2	0.27	0/1179	0.54	0/1584
12	F1	0.24	0/881	0.52	0/1189
12	F2	0.25	0/881	0.50	0/1189
13	G1	0.24	0/1246	0.54	0/1672
13	G2	0.25	0/1230	0.57	0/1649
14	H1	0.25	0/989	0.55	0/1326
14	H2	0.25	0/989	0.55	0/1326
15	I1	0.26	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.25	0/827	0.60	0/1117
16	J2	0.27	0/765	0.70	0/1033
17	K1	0.25	0/873	0.55	0/1180
17	K2	0.26	0/900	0.56	0/1215
18	L1	0.26	0/969	0.62	0/1300
18	L2	0.27	0/969	0.62	0/1300



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	M1	0.24	0/900	0.58	0/1204
19	M2	0.24	0/919	0.59	0/1226
20	N1	0.25	0/817	0.58	0/1088
20	N2	0.26	0/817	0.59	0/1088
21	O1	0.23	0/722	0.57	0/964
21	O2	0.23	0/722	0.59	0/964
22	P1	0.26	0/659	0.61	0/884
23	Q1	0.27	0/657	0.59	0/881
23	Q2	0.25	0/657	0.57	0/881
24	R1	0.25	0/635	0.58	0/849
24	R2	0.26	0/637	0.61	0/851
25	S1	0.25	0/680	0.52	0/915
25	S2	0.26	0/680	0.54	0/915
26	T1	0.25	0/676	0.52	0/895
27	U1	0.25	0/598	0.62	0/792
27	U2	0.25	0/592	0.58	0/785
28	V2	0.37	0/1552	0.97	8/2419 (0.3%)
29	W	0.34	1/1604 (0.1%)	0.79	1/2496 (0.0%)
30	W1	0.17	0/747	0.73	0/1161
31	X2	0.48	3/1628 (0.2%)	0.82	1/2526 (0.0%)
32	Y1	0.18	0/786	0.76	0/1216
33	Y2	0.34	1/1725 (0.1%)	0.78	1/2687 (0.0%)
34	Z1	0.28	0/76	0.34	0/101
35	a2	0.23	0/1033	0.47	0/1387
36	b2	0.26	0/2121	0.60	1/2852 (0.0%)
37	e2	0.25	0/1444	0.52	0/1937
38	g2	0.24	0/434	0.51	0/576
39	h2	0.25	0/1104	0.57	0/1474
40	i2	0.26	0/1122	0.51	0/1515
41	l2	0.24	0/380	0.63	0/498
42	o2	0.26	0/383	0.68	0/501
43	p	0.58	0/77	0.87	0/104
44	r2	0.25	0/901	0.60	0/1209
45	z2	0.26	0/589	0.55	0/779
All	All	0.22	7/203882 (0.0%)	0.70	33/307114 (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
10	D1	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
10	D2	0	1
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
43	p	0	1
All	All	0	10

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X2	1	G	OP3-P	-10.62	1.48	1.61
5	72	1	G	OP3-P	-10.59	1.48	1.61
33	Y2	1	G	OP3-P	-10.55	1.48	1.61
29	W	1	A	OP3-P	-10.52	1.48	1.61
31	X2	35	I	C5-C6	7.32	1.54	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	848	C	P-O3'-C3'	-9.46	108.34	119.70
7	A2	1532	U	P-O3'-C3'	-9.36	108.47	119.70
28	V2	43	U	P-O3'-C3'	-8.71	109.25	119.70
28	V2	41	G	P-O3'-C3'	-8.70	109.26	119.70
7	A2	1533	C	P-O3'-C3'	-8.11	109.96	119.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide
10	D2	104	ARG	Sidechain
16	J2	37	ARG	Sidechain
16	J2	48	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 PDB entries followed by that with respect to all EM entries.

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	
1	12	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	30
3	4	65/70 (93%)	50 (77%)	14 (22%)	1 (2%)	8	33
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	191 (83%)	35 (15%)	5 (2%)	5	26
8	B2	225/241 (93%)	188 (84%)	36 (16%)	1 (0%)	30	61
9	C1	211/233 (91%)	185 (88%)	24 (11%)	2 (1%)	14	44
9	C2	210/233 (90%)	184 (88%)	26 (12%)	0	100	100
10	D1	203/206 (98%)	181 (89%)	21 (10%)	1 (0%)	25	56
10	D2	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
11	E1	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
11	E2	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
12	F1	104/135 (77%)	104 (100%)	0	0	100	100
12	F2	104/135 (77%)	79 (76%)	22 (21%)	3 (3%)	3	21
13	G1	153/179 (86%)	150 (98%)	3 (2%)	0	100	100
13	G2	152/179 (85%)	119 (78%)	27 (18%)	6 (4%)	2	15
14	H1	127/130 (98%)	127 (100%)	0	0	100	100
14	H2	127/130 (98%)	127 (100%)	0	0	100	100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100	100
15	I2	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
16	J1	100/103 (97%)	91 (91%)	8 (8%)	1 (1%)	13	42
16	J2	90/103 (87%)	81 (90%)	8 (9%)	1 (1%)	12	40
17	K1	113/129 (88%)	97 (86%)	14 (12%)	2 (2%)	7	30
17	K2	116/129 (90%)	100 (86%)	14 (12%)	2 (2%)	7	31
18	L1	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	16	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
20	N1	98/101 (97%)	85 (87%)	13 (13%)	0	100	100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P1	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
23	Q1	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	1 (1%)	2 (3%)	4	23
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	34
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	9	34
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	5	24
27	U1	68/71 (96%)	57 (84%)	11 (16%)	0	100	100
27	U2	68/71 (96%)	59 (87%)	7 (10%)	2 (3%)	3	21
34	Z1	7/557 (1%)	7 (100%)	0	0	100	100
35	a2	130/234 (56%)	123 (95%)	7 (5%)	0	100	100
36	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
37	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
38	g2	50/55 (91%)	50 (100%)	0	0	100	100
39	h2	135/136 (99%)	135 (100%)	0	0	100	100
40	i2	147/149 (99%)	117 (80%)	27 (18%)	3 (2%)	6	28
41	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
42	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100
43	p	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
44	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
45	z2	74/85 (87%)	74 (100%)	0	0	100	100
All	All	6094/7240 (84%)	5593 (92%)	461 (8%)	40 (1%)	21	49

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
12	F2	38	ARG
13	G2	17	LYS
13	G2	18	PHE
13	G2	35	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 PDB entries followed by that with respect to all EM entries.

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	
1	12	67/68 (98%)	65 (97%)	2 (3%)	36	61
2	32	48/49 (98%)	47 (98%)	1 (2%)	48	70
3	4	60/62 (97%)	58 (97%)	2 (3%)	33	59
4	62	51/52 (98%)	51 (100%)	0	100	100
8	B	192/199 (96%)	191 (100%)	1 (0%)	86	91
8	B2	189/199 (95%)	184 (97%)	5 (3%)	41	65
9	C1	173/190 (91%)	172 (99%)	1 (1%)	84	90
9	C2	172/190 (90%)	171 (99%)	1 (1%)	84	90
10	D1	172/173 (99%)	169 (98%)	3 (2%)	56	74
10	D2	172/173 (99%)	171 (99%)	1 (1%)	84	90
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	126 (99%)	1 (1%)	79	87
14	H1	104/105 (99%)	104 (100%)	0	100	100
14	H2	104/105 (99%)	104 (100%)	0	100	100
15	I1	105/107 (98%)	105 (100%)	0	100	100
15	I2	106/107 (99%)	106 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	J1	89/90 (99%)	88 (99%)	1 (1%)	70	82
16	J2	82/90 (91%)	82 (100%)	0	100	100
17	K1	88/99 (89%)	87 (99%)	1 (1%)	70	82
17	K2	91/99 (92%)	91 (100%)	0	100	100
18	L1	103/104 (99%)	103 (100%)	0	100	100
18	L2	103/104 (99%)	103 (100%)	0	100	100
19	M1	93/96 (97%)	93 (100%)	0	100	100
19	M2	95/96 (99%)	95 (100%)	0	100	100
20	N1	83/84 (99%)	81 (98%)	2 (2%)	44	67
20	N2	83/84 (99%)	83 (100%)	0	100	100
21	O1	76/77 (99%)	76 (100%)	0	100	100
21	O2	76/77 (99%)	76 (100%)	0	100	100
22	P1	65/65 (100%)	65 (100%)	0	100	100
23	Q1	74/78 (95%)	74 (100%)	0	100	100
23	Q2	74/78 (95%)	74 (100%)	0	100	100
24	R1	64/65 (98%)	63 (98%)	1 (2%)	58	75
24	R2	64/65 (98%)	61 (95%)	3 (5%)	22	51
25	S1	72/79 (91%)	71 (99%)	1 (1%)	62	78
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	61 (94%)	4 (6%)	15	41
27	U1	60/61 (98%)	58 (97%)	2 (3%)	33	59
27	U2	59/61 (97%)	59 (100%)	0	100	100
34	Z1	8/461 (2%)	8 (100%)	0	100	100
35	a2	110/181 (61%)	109 (99%)	1 (1%)	75	85
36	b2	216/218 (99%)	216 (100%)	0	100	100
37	e2	149/150 (99%)	147 (99%)	2 (1%)	65	79
38	g2	47/49 (96%)	47 (100%)	0	100	100
39	h2	110/109 (101%)	110 (100%)	0	100	100
40	i2	114/114 (100%)	111 (97%)	3 (3%)	41	65
41	l2	38/38 (100%)	37 (97%)	1 (3%)	41	65
42	o2	35/103 (34%)	35 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	p	5/5 (100%)	4 (80%)	1 (20%)	1	4
44	r2	86/87 (99%)	86 (100%)	0	100	100
45	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5101/5932 (86%)	5060 (99%)	41 (1%)	77	87

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	T1	53	GLU
37	e2	178	ARG
26	T1	71	LYS
27	U1	66	ARG
40	i2	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
10	D2	85	ASN
12	F1	14	GLN
18	L2	29	GLN
12	F1	17	GLN
8	B2	89	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	63/64 (98%)	42 (66%)	8 (12%)
29	W	74/76 (97%)	24 (32%)	4 (5%)
30	W1	33/76 (43%)	8 (24%)	2 (6%)
31	X2	73/77 (94%)	26 (35%)	5 (6%)
32	Y1	32/76 (42%)	4 (12%)	2 (6%)
33	Y2	75/76 (98%)	22 (29%)	2 (2%)
5	71	28/2904 (0%)	4 (14%)	0
5	72	2899/2904 (99%)	456 (15%)	30 (1%)
6	82	119/120 (99%)	21 (17%)	4 (3%)
7	A1	1538/1542 (99%)	452 (29%)	39 (2%)
7	A2	1533/1542 (99%)	400 (26%)	33 (2%)
All	All	6467/9457 (68%)	1459 (22%)	129 (1%)

5 of 1459 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1906	G
5	71	1907	G
5	71	1929	G
5	71	1930	G
5	72	10	A

5 of 129 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	W	18	G
30	W1	43	C
7	A1	438	U
7	A1	428	G
31	X2	22	A

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

73 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	$\# Z  > 2$
30	PSU	W1	32	30	18,21,22	4.67	8 (44%)	22,30,33	1.79	5 (22%)
7	2MG	A2	1516	7	18,26,27	2.84	7 (38%)	16,38,41	1.36	3 (18%)
31	3AU	X2	48	31	24,28,29	2.84	7 (29%)	33,40,43	1.31	3 (9%)
32	CM0	Y1	34	32	23,26,27	3.74	6 (26%)	27,37,40	1.50	2 (7%)
7	2MG	A1	966	7	18,26,27	2.86	7 (38%)	16,38,41	1.41	3 (18%)
7	UR3	A1	1498	7	19,22,23	2.79	8 (42%)	26,32,35	1.31	3 (11%)
5	OMG	72	2251	29,5	18,26,27	2.84	7 (38%)	19,38,41	1.52	4 (21%)
30	G7M	W1	46	30	20,26,27	2.81	7 (35%)	17,39,42	1.12	1 (5%)
5	PSU	72	2457	5	18,21,22	4.64	8 (44%)	22,30,33	1.91	5 (22%)
31	4SU	X2	8	31	18,21,22	3.79	7 (38%)	26,30,33	2.26	4 (15%)
7	2MG	A1	1516	7	18,26,27	2.86	7 (38%)	16,38,41	1.36	3 (18%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	G7M	Y2	46	33	20,26,27	2.81	8 (40%)	17,39,42	1.08	1 (5%)
7	2MG	A2	966	7	18,26,27	2.87	7 (38%)	16,38,41	1.33	3 (18%)
7	5MC	A1	1407	7	18,22,23	4.06	7 (38%)	26,32,35	1.00	2 (7%)
29	5MU	W	54	29	19,22,23	7.21	7 (36%)	28,32,35	3.32	9 (32%)
7	5MC	A2	1407	7	18,22,23	4.03	7 (38%)	26,32,35	0.98	1 (3%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
7	4OC	A1	1402	7	20,23,24	3.24	8 (40%)	26,32,35	0.91	1 (3%)
29	H2U	W	16	29	18,21,22	3.06	5 (27%)	21,30,33	1.90	5 (23%)
33	5MU	Y2	54	33	19,22,23	7.19	7 (36%)	28,32,35	3.33	9 (32%)
7	4OC	A2	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.91	1 (3%)
31	PSU	X2	56	31	18,21,22	4.70	8 (44%)	22,30,33	1.80	5 (22%)
5	2MG	72	1835	5	18,26,27	2.81	7 (38%)	16,38,41	1.43	4 (25%)
5	5MC	72	1962	5	18,22,23	4.03	7 (38%)	26,32,35	1.04	2 (7%)
5	PSU	72	2605	5	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
5	H2U	72	2449	49,5	18,21,22	3.04	5 (27%)	21,30,33	2.03	5 (23%)
5	5MU	72	747	5	19,22,23	7.17	7 (36%)	28,32,35	3.47	10 (35%)
7	5MC	A1	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.01	2 (7%)
7	5MC	A2	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.00	2 (7%)
5	1MG	72	745	5	18,26,27	2.76	6 (33%)	19,39,42	1.45	4 (21%)
5	6MZ	72	2030	5	18,25,26	2.08	3 (16%)	16,36,39	2.29	3 (18%)
29	H2U	W	20	29	18,21,22	3.06	5 (27%)	21,30,33	2.01	5 (23%)
30	MIA	W1	37	30	24,31,32	2.36	3 (12%)	26,44,47	2.68	7 (26%)
29	G7M	W	46	29	20,26,27	2.80	7 (35%)	17,39,42	1.13	1 (5%)
33	PSU	Y2	55	33	18,21,22	4.66	8 (44%)	22,30,33	1.87	5 (22%)
5	2MG	72	2445	5	18,26,27	2.84	7 (38%)	16,38,41	1.39	3 (18%)
31	G7M	X2	47	31	20,26,27	2.83	7 (35%)	17,39,42	1.24	1 (5%)
5	G7M	72	2069	5	20,26,27	2.80	8 (40%)	17,39,42	1.05	1 (5%)
32	6MZ	Y1	37	32	18,25,26	2.05	2 (11%)	16,36,39	2.46	4 (25%)
29	PSU	W	32	29	18,21,22	4.64	8 (44%)	22,30,33	1.87	5 (22%)
31	H2U	X2	17	31	18,21,22	3.06	5 (27%)	21,30,33	2.00	5 (23%)
31	5MU	X2	55	31	19,22,23	7.20	7 (36%)	28,32,35	3.31	9 (32%)
7	2MG	A1	1207	7	18,26,27	2.86	7 (38%)	16,38,41	1.35	3 (18%)
5	OMC	72	2498	49,5	19,22,23	3.29	8 (42%)	26,31,34	0.78	0
31	2MA	X2	38	31	19,25,26	3.65	6 (31%)	21,37,40	3.63	3 (14%)
5	3TD	72	1915	5	19,22,23	4.05	7 (36%)	21,32,35	1.74	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	6MZ	72	1618	5	18,25,26	2.03	2 (11%)	16,36,39	2.23	4 (25%)
7	UR3	A2	1498	7	19,22,23	2.77	8 (42%)	26,32,35	1.31	3 (11%)
5	PSU	72	746	49,5	18,21,22	4.70	8 (44%)	22,30,33	1.79	5 (22%)
31	RSP	X2	33	31	17,21,22	4.11	7 (41%)	22,30,33	0.80	0
7	MA6	A2	1519	7	18,26,27	1.05	2 (11%)	19,38,41	3.41	3 (15%)
29	PSU	W	55	29	18,21,22	4.68	8 (44%)	22,30,33	1.85	5 (22%)
31	H2U	X2	21	31	18,21,22	3.07	5 (27%)	21,30,33	2.05	5 (23%)
30	4SU	W1	8	30	18,21,22	3.81	7 (38%)	26,30,33	2.22	4 (15%)
7	MA6	A2	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.44	3 (15%)
29	H2U	W	17	29	18,21,22	3.07	5 (27%)	21,30,33	2.00	5 (23%)
32	7MG	Y1	46	32	22,26,27	3.91	10 (45%)	29,39,42	2.09	9 (31%)
7	2MG	A2	1207	7	18,26,27	2.86	7 (38%)	16,38,41	1.40	3 (18%)
30	PSU	W1	39	30	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
5	2MA	72	2503	5	19,25,26	3.59	6 (31%)	21,37,40	3.63	4 (19%)
7	MA6	A1	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.46	3 (15%)
5	5MU	72	1939	5	19,22,23	7.17	7 (36%)	28,32,35	3.46	10 (35%)
5	PSU	72	2504	49,5	18,21,22	4.68	8 (44%)	22,30,33	1.84	5 (22%)
5	PSU	72	2580	5	18,21,22	4.66	8 (44%)	22,30,33	1.83	6 (27%)
29	MIA	W	37	29	24,31,32	2.32	3 (12%)	26,44,47	2.62	7 (26%)
7	MA6	A1	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.45	3 (15%)
7	G7M	A2	527	7	20,26,27	2.80	8 (40%)	17,39,42	1.01	1 (5%)
33	H2U	Y2	17	33	18,21,22	3.08	5 (27%)	21,30,33	2.01	5 (23%)
5	PSU	72	2604	5	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
5	3TD	71	1915	5	19,22,23	4.11	7 (36%)	21,32,35	1.64	2 (9%)
29	4SU	W	8	29	18,21,22	3.78	7 (38%)	26,30,33	2.25	5 (19%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
7	G7M	A1	527	7	20,26,27	2.80	7 (35%)	17,39,42	1.04	1 (5%)

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
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	3AU	X2	48	31	-	6/16/34/35	0/2/2/2
32	CM0	Y1	34	32	-	4/12/30/31	0/2/2/2
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
5	OMG	72	2251	29,5	-	3/5/27/28	0/3/3/3
30	G7M	W1	46	30	-	3/3/25/26	0/3/3/3
5	PSU	72	2457	5	-	0/7/25/26	0/2/2/2
31	4SU	X2	8	31	-	2/7/25/26	0/2/2/2
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
33	G7M	Y2	46	33	-	2/3/25/26	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
29	5MU	W	54	29	-	2/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
7	4OC	A1	1402	7	-	1/9/29/30	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
33	5MU	Y2	54	33	-	2/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
31	PSU	X2	56	31	-	1/7/25/26	0/2/2/2
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
5	H2U	72	2449	49,5	-	0/7/38/39	0/2/2/2
5	5MU	72	747	5	-	1/7/25/26	0/2/2/2
7	5MC	A1	967	7	-	1/7/25/26	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
29	H2U	W	20	29	-	1/7/38/39	0/2/2/2
30	MIA	W1	37	30	-	6/11/33/34	0/3/3/3
29	G7M	W	46	29	-	3/3/25/26	0/3/3/3
33	PSU	Y2	55	33	-	0/7/25/26	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
31	G7M	X2	47	31	-	3/3/25/26	0/3/3/3
5	G7M	72	2069	5	-	3/3/25/26	0/3/3/3
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
29	PSU	W	32	29	-	0/7/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	H2U	X2	17	31	-	6/7/38/39	0/2/2/2
31	5MU	X2	55	31	-	2/7/25/26	0/2/2/2
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
5	OMC	72	2498	49,5	-	2/9/27/28	0/2/2/2
31	2MA	X2	38	31	-	3/3/25/26	0/3/3/3
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
5	PSU	72	746	49,5	-	1/7/25/26	0/2/2/2
31	RSP	X2	33	31	-	1/7/25/26	0/2/2/2
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
29	PSU	W	55	29	-	0/7/25/26	0/2/2/2
31	H2U	X2	21	31	-	1/7/38/39	0/2/2/2
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
7	MA6	A2	1518	7	-	3/7/29/30	0/3/3/3
29	H2U	W	17	29	-	2/7/38/39	0/2/2/2
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
5	2MA	72	2503	5	-	0/3/25/26	0/3/3/3
7	MA6	A1	1519	7	-	4/7/29/30	0/3/3/3
5	5MU	72	1939	5	-	0/7/25/26	0/2/2/2
5	PSU	72	2504	49,5	-	0/7/25/26	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
29	MIA	W	37	29	-	3/11/33/34	0/3/3/3
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3
7	G7M	A2	527	7	-	3/3/25/26	0/3/3/3
33	H2U	Y2	17	33	-	7/7/38/39	0/2/2/2
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
29	4SU	W	8	29	-	2/7/25/26	0/2/2/2
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3

The worst 5 of 476 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	747	5MU	C4-C5	21.41	1.80	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	1939	5MU	C4-C5	21.37	1.80	1.44
31	X2	55	5MU	C4-C5	21.31	1.80	1.44
29	W	54	5MU	C4-C5	21.22	1.80	1.44
33	Y2	54	5MU	C4-C5	21.21	1.80	1.44

The worst 5 of 286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2503	2MA	C1'-N9-C4	14.74	152.54	126.64
31	X2	38	2MA	C1'-N9-C4	14.73	152.52	126.64
7	A1	1519	MA6	N1-C6-N6	-12.61	103.79	117.06
7	A1	1518	MA6	N1-C6-N6	-12.57	103.83	117.06
7	A2	1519	MA6	N1-C6-N6	-12.53	103.87	117.06

There are no chirality outliers.

5 of 112 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	Y1	37	6MZ	N1-C6-N6-C9
33	Y2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	17	H2U	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C6
33	Y2	17	H2U	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 303 ligands modelled in this entry, 299 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	$\# Z  > 2$
47	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.51	0
50	ALA	Y2	102	33	3,4,5	1.17	0	2,4,6	3.10	1 (50%)
48	SPD	72	3003	-	9,9,9	0.33	0	8,8,8	0.86	0
47	PUT	72	3002	-	5,5,5	0.25	0	4,4,4	0.55	0

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
47	PUT	72	3001	-	-	1/3/3/3	-
50	ALA	Y2	102	33	-	0/0/2/4	-
48	SPD	72	3003	-	-	0/7/7/7	-
47	PUT	72	3002	-	-	0/3/3/3	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
50	Y2	102	ALA	O-C-CA	-4.38	110.42	124.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 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.