



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 31, 2017 – 12:43 PM EST

PDB ID : 3JBV
EMDB ID: : EMD-6486
Title : Mechanisms of Ribosome Stalling by SecM at Multiple Elongation Steps
Authors : Zhang, J.; Pan, X.J.; Yan, K.G.; Sun, S.; Gao, N.; Sui, S.F.
Deposited on : 2015-10-16
Resolution : 3.32 Å(reported)
Based on PDB ID : 4V7T

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

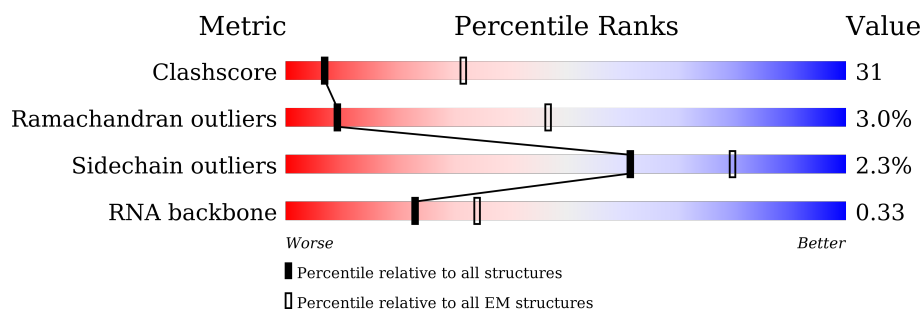
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1542	42% 39% 17% .
2	B	241	57% 31% . 10%
3	C	233	53% 33% . 12%
4	D	206	56% 43%
5	E	167	55% 31% . 10%
6	F	131	48% 28% 24%
7	G	156	67% 27% . .
8	H	130	66% 33% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	V	76	
23	W	75	
24	X	11	
25	0	78	
26	1	63	
27	2	59	
28	3	57	
29	4	55	
30	6	46	
31	7	65	
32	8	38	
33	a	120	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	b	2904	
35	c	273	
36	i	142	
37	d	209	
38	e	201	
39	f	179	
40	g	177	
41	h	149	
42	j	142	
43	k	123	
44	l	144	
45	m	136	
46	n	127	
47	o	117	
48	p	115	
49	q	118	
50	r	103	
51	s	110	
52	t	100	
53	u	104	
54	w	94	
55	y	85	
56	z	27	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145911 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 RNA chain called RNA (1530-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	113	Total	C	N	O	S	0	0
			876	541	177	155	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	79	ARG	GLN	ENGINEERED MUTATION	UNP P0ADZ4

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	76	Total	C	N	O	P	0	0
			1620	723	290	532	75		

- Molecule 23 is a RNA chain called RNA (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	P	0	0
			1599	713	287	525	74		

- Molecule 24 is a RNA chain called RNA (5'-R(P*CP*UP*GP*GP*CP*CP*CP*UP*CP*A P*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	11	Total	C	N	O	P	0	0
			231	103	39	78	11		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 33 is a RNA chain called RNA (118-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	117	Total	C	N	O	P	0	0
			2506	1116	459	814	117		

- Molecule 34 is a RNA chain called RNA (2903-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 35 is a protein called 50S ribosomal protein L2.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	134	Total	C	N	O	S	0	0
			976	614	169	187	6		

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 43 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 44 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 45 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	135	Total	C	N	O	S	0	0
			1063	680	201	176	6		

- Molecule 46 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 47 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	o	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 48 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 49 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 50 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 51 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 52 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 53 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

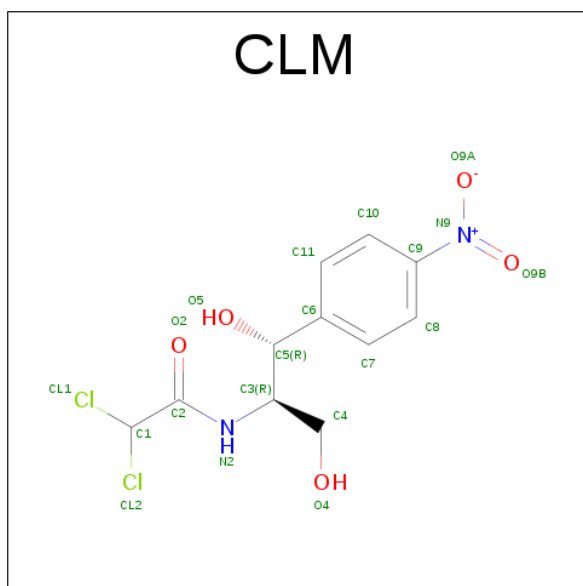
- Molecule 55 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	y	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 56 is a protein called Secretion monitor.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	z	27	Total	C	N	O	0	0
			211	134	35	42		

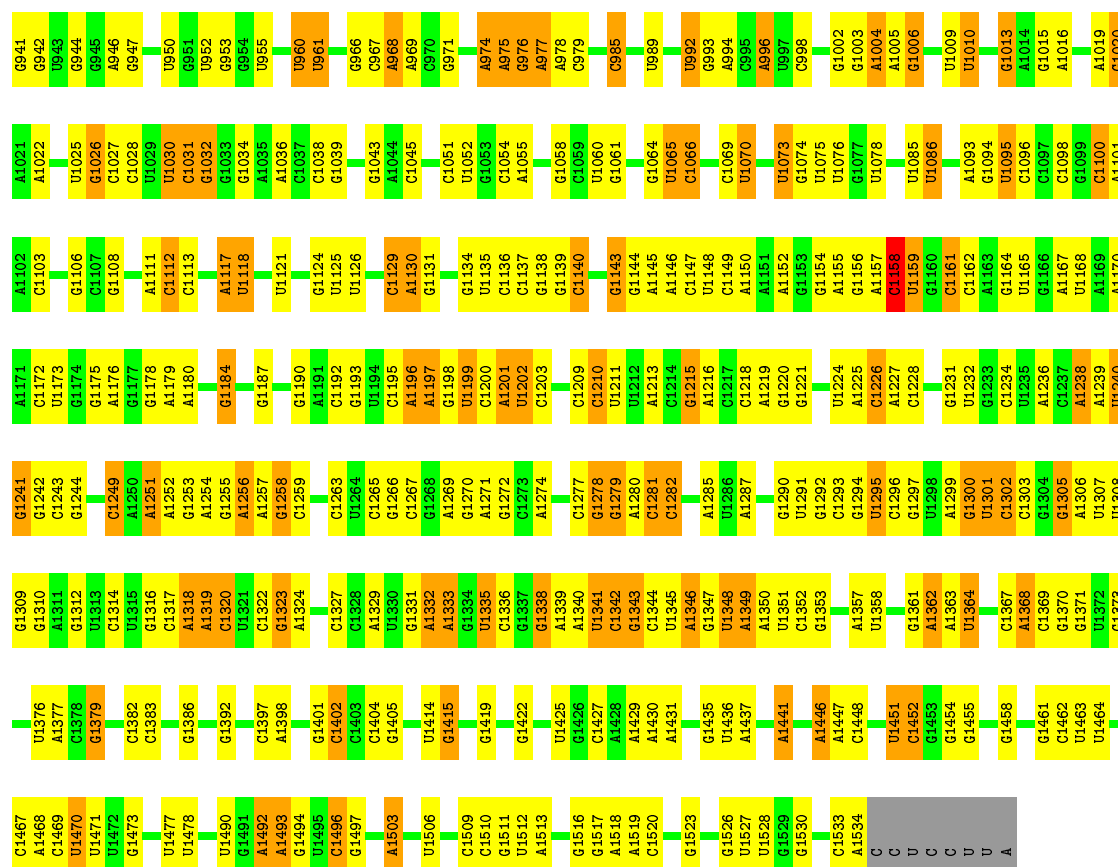
- Molecule 57 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					AltConf
57	b	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

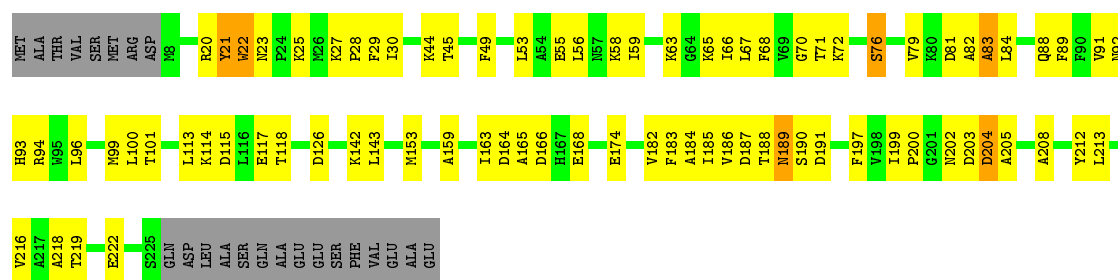
- Molecule 1: RNA (1530-MER)





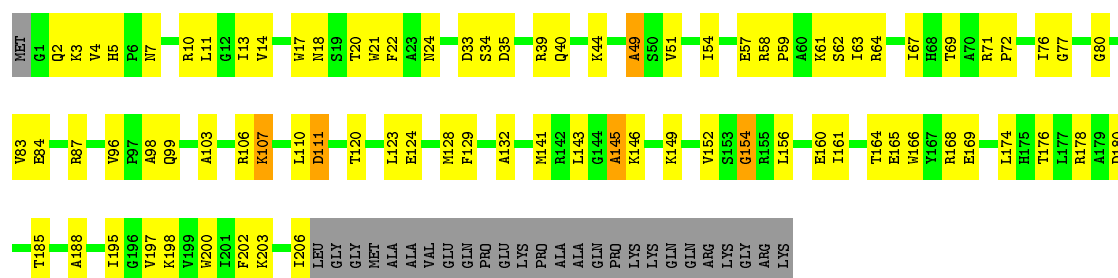
• Molecule 2: 30S ribosomal protein S2

Chain B: 57% 31% 10%

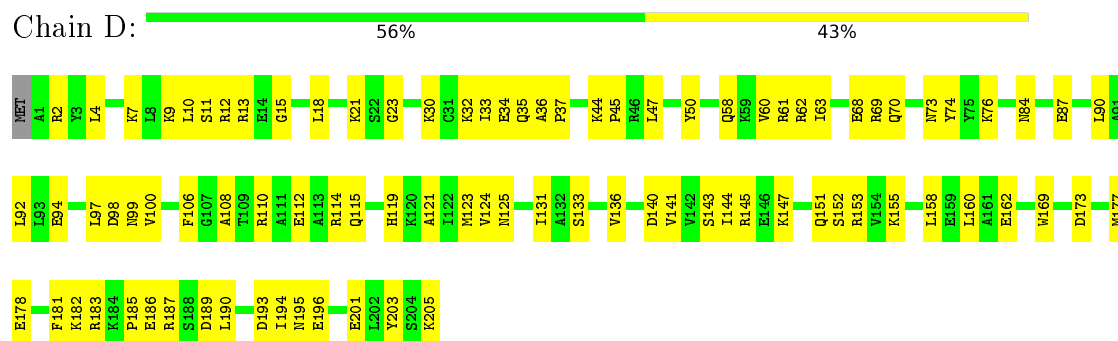


• Molecule 3: 30S ribosomal protein S3

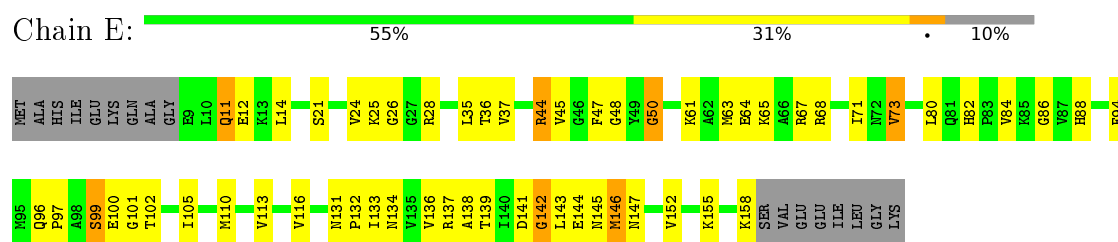
Chain C: 53% 33% 12%



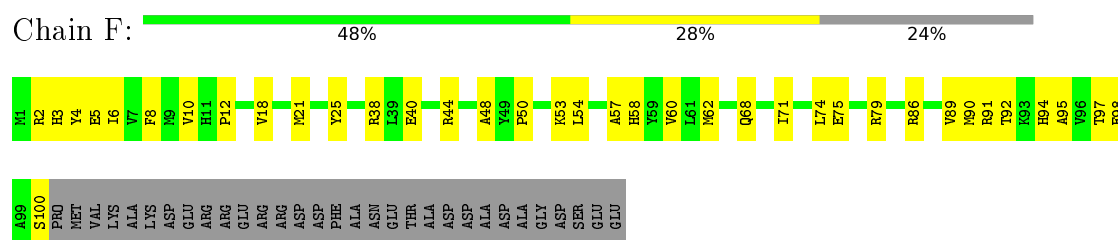
- Molecule 4: 30S ribosomal protein S4



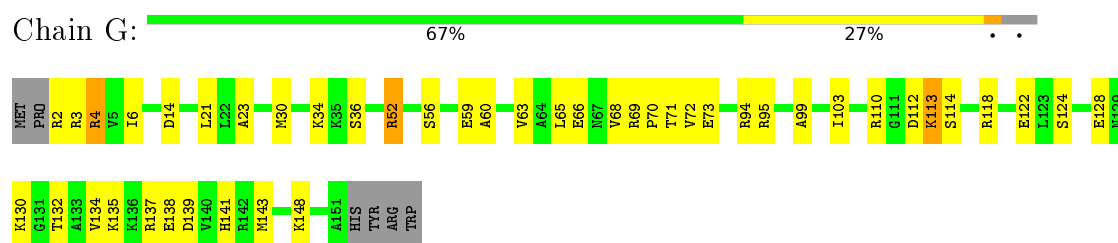
- Molecule 5: 30S ribosomal protein S5



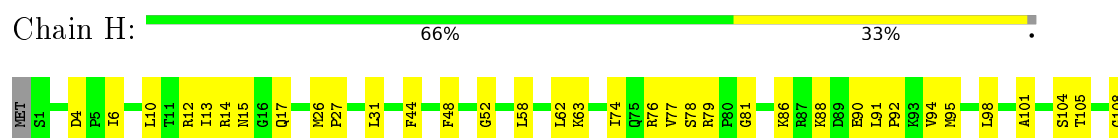
- Molecule 6: 30S ribosomal protein S6

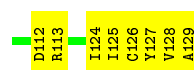


- Molecule 7: 30S ribosomal protein S7



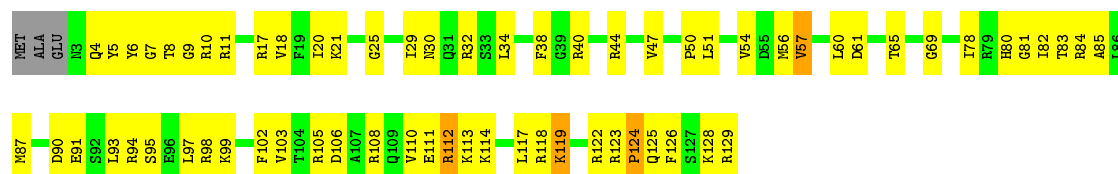
- Molecule 8: 30S ribosomal protein S8





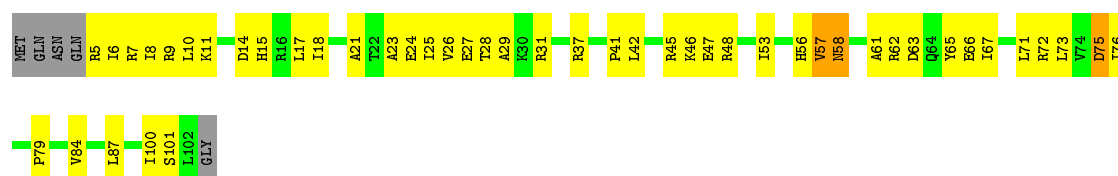
• Molecule 9: 30S ribosomal protein S9

Chain I: 47% 48% ..



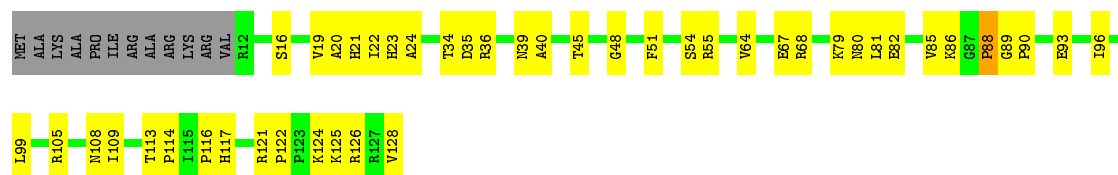
• Molecule 10: 30S ribosomal protein S10

Chain J: 50% 43% 5%



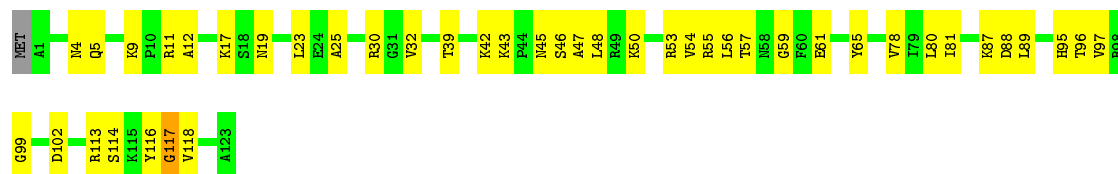
• Molecule 11: 30S ribosomal protein S11

Chain K: 56% 34% 9%



• Molecule 12: 30S ribosomal protein S12

Chain L: 65% 34% ..



• Molecule 13: 30S ribosomal protein S13

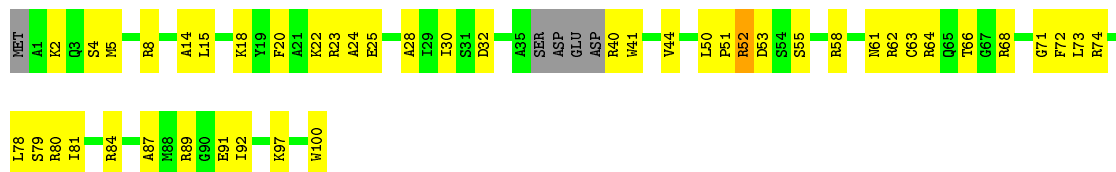
Chain M: 53% 42% .





- Molecule 14: 30S ribosomal protein S14

Chain N: 50% 44% 5%



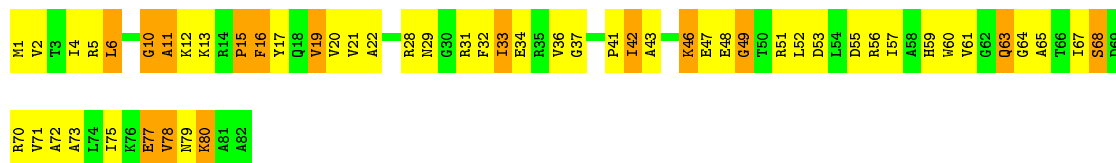
- Molecule 15: 30S ribosomal protein S15

Chain O: 67% 31%



- Molecule 16: 30S ribosomal protein S16

Chain P: 34% 48% 18%



- Molecule 17: 30S ribosomal protein S17

Chain Q: 61% 33% 5%



- Molecule 18: 30S ribosomal protein S18

Chain R: 48% 25% 27%



- Molecule 19: 30S ribosomal protein S19

Chain S: 51% 34% 14%



LYS
ALA
LYS
LYS
LYS

- Molecule 20: 30S ribosomal protein S20

Chain T:  69% 29% .

MET ALA I2 R9 Q12 A16 H19 M27 E28 F30 T29 I31 K32 K33 V34 Y35 I38 F50 M53 Q54 P55 R59 H67 K68 N69 K70 R73 A76 N77 L78 T79 I82 A86

- Molecule 21: 30S ribosomal protein S21

Chain U:  34% 34% 28% .

MET PRO VAL I3 K4 V5 R6 E7 P10 G10 P11 A14 I15 R16 K19 E23 K24 A25 G26 V27 L28 A29 E30 V31 R32 R33 R34 E35 E38 K39 R44 K45 R46 A47 K48 A49 S50 K53 ARG HIS ALA LYS LYS LEU ALA ARG GLU ASN ALA ARG THR ARG LEU TYR

- Molecule 22: RNA (76-MER)

Chain V:  14% 43% 41% .

G1 C2 C3 C4 G5 G6 A7 U8 A9 G10 C11 U12 G15 U16 C17 G18 G19 U20 A21 A22 G23 A23 G24 C25 A26 G27 G28 G29 G30 U33 A34 G35 G36 A37 A38 U39 C40 C41 C42 C43 G44 G45 G46 U47 C48 C49 U50 U51 G52 G53 U54 U55 C56 G57 A58 U59 U60 C61 C62 G63 A64 G65 U66 C67 G68 G69 G70 G71 C72 A73 C74 C75 A76

- Molecule 23: RNA (75-MER)

Chain W:  31% 49% 19% .


C1 G2 G3 C6 G7 U8 A9 C13 A14 G15 C16 U17 G18 G19 U20 A21 G22 C28 C31 U32 A33 G34 C35 C36 G37 U38 G39 U40 C41 G42 G43 G44 G45 G46 U47 C48 G49 G50 A51 G52 U55 C56 A57 A58 A59 U60 C61 C62 C66 G67 U68 G69 C70 C71 G72 A73 C74 A75

- Molecule 24: RNA (5'-R(P*CP*UP*GP*GP*CP*CP*CP*UP*CP*AP*A)-3')

Chain X:  27% 64% 9%


G12 U13 G14 G15 C16 C17 U18 C20 A21 A22

- Molecule 25: 50S ribosomal protein L28

Chain 0:  90% 8% ..

MET S2 R11 M17 T48 R57 V67 L68 L71 Y78

- Molecule 26: 50S ribosomal protein L29

Chain 1:  84% 13% ..




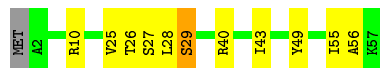
- Molecule 27: 50S ribosomal protein L30

Chain 2:  86% 8% ..




- Molecule 28: 50S ribosomal protein L32

Chain 3:  79% 18% ..



- Molecule 29: 50S ribosomal protein L33

Chain 4:  85% 5% 9%




- Molecule 30: 50S ribosomal protein L34

Chain 6:  89% 7% .



- Molecule 31: 50S ribosomal protein L35

Chain 7:  89% 9% .



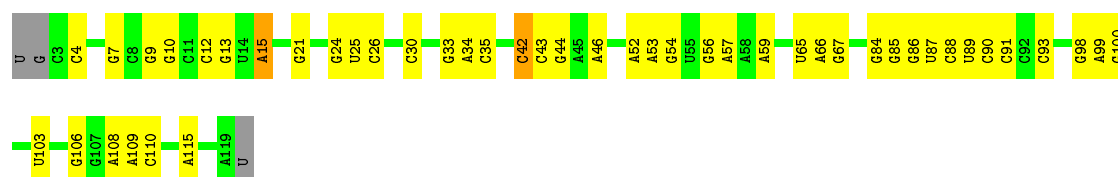
- Molecule 32: 50S ribosomal protein L36

Chain 8:  87% 13%



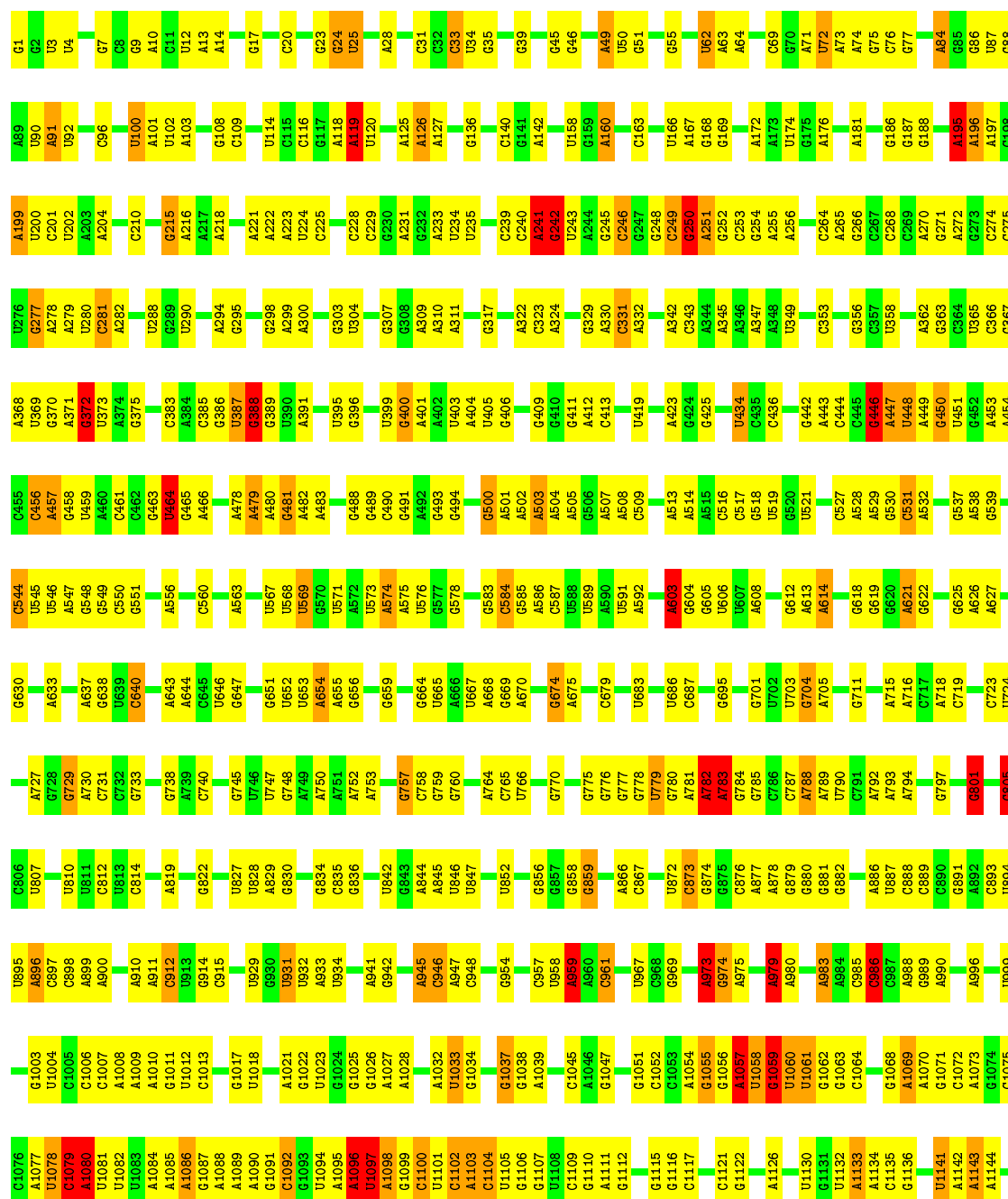
- Molecule 33: RNA (118-MER)

Chain a:  59% 37% ..

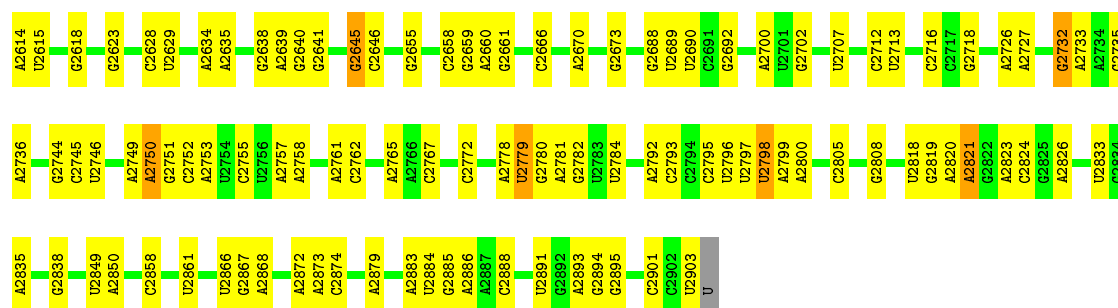


• Molecule 34: RNA (2903-MER)

Chain b: 55% 38% 5%



A2450	A2534	G2279	C2175	A2108	C2021	G1929	U1820	C1728	G1531	G1521	G1424	G1331	A1241	A1151
A2453	G2535	G2280	A2176	U2109	U2022	G1930	G1824	U1729	G1631	A1522	G1425	G1332	A1242	A1155
G2454	G2536	A2281	C2178	U2111	G2024	U1931	A1824	C1731	G1632	G1523	G1426	G1338	C1243	A1156
C2456	G2544	G2282	C2179	G2112	C2025	A1936	U1827	G1732	G1633	G1524	A1427	G1339	A1244	
U2457	G2545	A2284	A2183	U2113	U2026	A1937	G1828	G1733	A1634	G1529	G1444	U1340	A1247	G1163
G2458	A2547	C2285	U2184	A2114	G2027	A1938	A1829	A1735	A1637	G1530	G1449	A1341	G1248	G1168
A2459	C2551	G2286	U2185	G2116	A2030	U1939	C1833	A1746	G1644	A1535	G1450	G1343	U1249	
C2465	C2554	A2287	G2190	U2117	A2031	U1940	G1839		G1645	A1536	G1451	U1344	A1169	G1170
C2466	U2554	A2288	A2191	U2118	G2032	C1941	G1839		C1646	A1537	C1451	U1345	A1171	C1171
C2467	G2555	G2289	A2192	A2119	A2033	C1942		G1750	U1647	G1538	A1452	G1346	C1172	C1172
G2470	G2556		G2193	G2120	U1943	U1943	G1842		G1648	U1539	A1453	A1347	U1173	U1173
A2471	G2557		A2188	G2121	C2035	U1944		A1754	G1649	U1542	G1454	C1348	G1256	U1174
G2472	C2562	A2297	U2189	U2122	C2036	A1952	G1845	A1755	A1654	G1455	C1455	C1349	A1175	A1175
U2473	U2562	A2298	A2198	G2123	A2042	A1953	G1846	A1756	A1655	U1458	U1352	U1352	U1176	U1176
A2474	C2563	G2304	A2199	C2124	C2043	G1954	A1847	A1757	C1655	G1459	A1353	A1353	C1178	C1178
C2475	A2564	A2204	G2204	G2125	C2044	U1955	A1848	U1758	C1656	A1265	U1265	A1354	A1179	A1179
G2476	G2565	U2305	G2203	A2126	C2045	C1958	G1849	A1759	U1657	U1266	G1266	G1355	U1180	U1180
A2477	A2566	G2128	A2204	G2127	G2046	G1959	A1853	C1761	G1658	C1267	U1267	U1355	U1181	
G2478	G2567	G2307	U2210	G2129	G2046	G1960	A1857	A1762	G1659	A1268	U1268	A1365	U1184	U1184
	A2478	G2308	A2211	U2130	G2049	C1961	G1857	G1763	G1660	U1562	U1467	A1365	G1185	G1185
			A2212	U2131	C2050	G1962	G1857	C1764	G1663	A1271	U1468	U1352	A1186	A1186
G2481	U2571	A2311	U2213	U2132	A2051	U1963	G1862	U1765	G1667	C1272	A1469	A1353	G1187	G1187
A2482	C2572	C2312	C2214	G2133	C2051	G1964	A1866	G1766	A1668	A1274	U1470	C1370	A1274	U1188
G2483	G2574	U2312	C2214	G2133	C2055	C1965	G1867		G1669	G1275	A1477	G1374	A1275	
G2484	G2575	G2316	C2215	U2139	G2056	A1966	C1868	A1772	C1670	A1276	A1477	G1374	A1276	
			G2218		G2057	C1967	G1869	A1773	U1671	G1276	G1478			G1195
G2488	A2577	G2319	A2225	A2142	A2060	A1970	G1869	C1774	U1672	G1280				G1197
U2489	G2578	U2320	A2225	C2143	G2061	A1971	A1870	U1775	G1673	A1287				C1200
G2490		U2321	C2238	G2144	A2062	G1971	A1871	U1776	G1674	A1287				U1201
U2491	G2582	A2322	G2239	C2145	C2063	G1972	G1875	U1777	U1578	U1294				G1202
	C2583	G2323	G2239	C2146	C2063	A1977	A1876	U1778	A1677	C1295				U1203
C2496	U2584	U2324	U2243	A2147	C2066	G1977	A1876	U1779	A1677	G1296				A1204
A2497	G2585	G2325	U2243	G2148	C2066	G1980	A1877	A1780	A1677	A1295				A1204
C2498	U2586	C2326	U2243	U2149	G2067	G1981	A1877	A1781	A1689	G1299				G1206
G2499		A2327	C2248	G2152	U2068	A1981	A1885	U1781	A1689	C1386				
U2500	G2589	G2327	U2249	G2152	G2069	U1982	A1890	A1783	C1690	G1387				U1209
C2501	A2584	G2330	G2250	C2153	A2070	U1989	A1890	A1784	C1691	A1301				G1210
G2502	C2425	G2331	G2251	G2153	G2076	G1989	A1896	U1785	U1683	A1302				U1211
A2503	U2593	C2332	G2252	G2156	U2076	C1990	G1896	A1786	C1694	A1306				G1212
C2594	G2594	A2333	C2255	G2157	A2077	U1991	A1901	A1787	A1698	C1306				
G2504	U2595	G2334	G2256	A2158	G2077	G1992	C1902	C1800	C1699	G1310				G1218
C2505	G2596	A2335	G2256	G2159	A2080	U1993	C1902	A1801	A1700	G1311				
U2506	G2597	A2336	U2257	C2160	G2087	C1996	C1905	A1802	A1701	U1312				U1222
G2507				C2161	G2087	C1996	G1906	A1802	A1701	G1312				G1223
G2508	A2600	A2340	C2261	C2162	U2092	C1997	A1906	A1805	G1702	U1313				U1224
	C2601	A2343	U2271	A2163	U2092	C1997	C1906	A1805	G1703	A1502				G1225
A2513	G2602	G2345	U2265	C2163	A2095	G2004	C1908	A1806	C1704	A1503				A1226
G2517	G2603	A2346	A2266	C2165	A2095	A2005	C1908	G1807	A1705	A1504				G1227
A2518	U2604	C2347	A2267	U2166	C2096	C2006	U1911	A1808	C1706	U1415				
U2519			A2268	U2167	A2097	U2007	A1912	A1809	G1710	C1320				G1232
	G2607	C2350		G2168	U2098	U2098	A1913	A1810	G1710	A1514				G1232
	G2608		G2271	A2169	U2098	G2010	A1913	A1810	G1710	A1514				G1232
G2608	U2609	G2353	U2272	A2170	C2103	U2011	U1915	A1811	A1713	A1507				G1236
G2610		C2354	A2273	C2104	U2103	U2011	U1915	A1814	A1713	A1508				G1236
C2611	U2610	G2447	A2274	U2172	U2105	A2014	C1924	A1814	U1714	A1509				A1237
G2612	U2611	G2448	A2275	U2173	U2106	A2014	C1924	A1814	G1715	A1511				G1238
G2613	C2612	C2357	C2275	C2174	U2106	U2014	C1924	A1814	U1716	C1512				G1239
			C2276	A2174	C2107	C2020	A1928	A1819						U1240



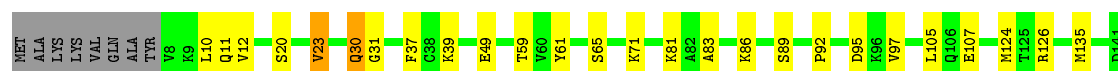
- Molecule 35: 50S ribosomal protein L2

Chain c: 96%



- Molecule 36: 50S ribosomal protein L9

Chain i: 76%



- Molecule 37: 50S ribosomal protein L11

Chain d: 97%



- Molecule 38: 50S ribosomal protein L3

Chain e: 94%



- Molecule 39: 50S ribosomal protein L4

Chain f: 93%



- Molecule 40: 50S ribosomal protein L5

Chain g: 95%



- Molecule 41: 50S ribosomal protein L6

Chain h:  97% ..



- Molecule 42: 50S ribosomal protein L13

Chain j:  96% .




- Molecule 43: 50S ribosomal protein L14

Chain k:  95% ..



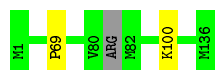
- Molecule 44: 50S ribosomal protein L15

Chain l:  92% 8%




- Molecule 45: 50S ribosomal protein L16

Chain m:  98% ..



- Molecule 46: 50S ribosomal protein L17

Chain n:  91% . 6%



- Molecule 47: 50S ribosomal protein L18

Chain o:  93% 6% .



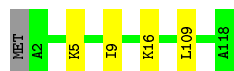
- Molecule 48: 50S ribosomal protein L19

Chain p:  95% ..



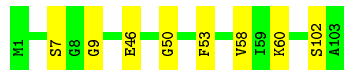
- Molecule 49: 50S ribosomal protein L20

Chain q:  96% ..



- Molecule 50: 50S ribosomal protein L21

Chain r:  92% 8%




- Molecule 51: 50S ribosomal protein L22

Chain s:  95% 5%




- Molecule 52: 50S ribosomal protein L23

Chain t:  86% 7% 7%



- Molecule 53: 50S ribosomal protein L24

Chain u:  84% 14% .




- Molecule 54: 50S ribosomal protein L25

Chain w:  98% .



- Molecule 55: 50S ribosomal protein L27

Chain y:  87% 12%



● Molecule 56: Secretion monitor



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	60354	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	3500	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	37878	Depositor
Image detector	GATAN K2 Summit (4K 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: CLM

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.47	0/36762	0.79	8/57350 (0.0%)
10	J	0.29	0/796	0.56	0/1077
11	K	0.28	0/893	0.52	0/1205
12	L	0.32	0/969	0.56	0/1300
13	M	0.27	0/884	0.49	0/1181
14	N	0.30	0/785	0.50	0/1043
15	O	0.30	0/724	0.48	0/966
16	P	0.29	0/659	0.49	0/884
17	Q	0.31	0/657	0.49	0/881
18	R	0.29	0/462	0.50	0/621
19	S	0.30	0/652	0.51	0/877
2	B	0.28	0/1735	0.50	0/2338
20	T	0.31	0/671	0.49	0/888
21	U	0.29	0/430	0.60	0/570
22	V	0.33	0/1810	0.80	3/2821 (0.1%)
23	W	0.35	1/1786 (0.1%)	0.92	6/2784 (0.2%)
24	X	0.87	1/256 (0.4%)	0.81	0/394
25	0	0.41	0/635	0.76	1/848 (0.1%)
26	1	0.35	0/502	0.63	0/667
27	2	0.39	0/453	0.64	0/605
28	3	0.42	0/450	0.80	1/599 (0.2%)
29	4	0.38	0/416	0.61	0/554
3	C	0.32	0/1651	0.53	0/2225
30	6	0.48	0/380	0.86	0/498
31	7	0.40	0/513	0.65	0/676
32	8	0.40	0/303	0.77	0/397
33	a	0.45	1/2802 (0.0%)	0.89	4/4369 (0.1%)
34	b	0.59	84/69800 (0.1%)	1.02	432/108892 (0.4%)
35	c	0.42	0/2121	0.76	2/2852 (0.1%)
36	i	0.24	0/989	0.48	0/1334
37	d	0.39	0/1586	0.67	2/2134 (0.1%)
38	e	0.39	0/1571	0.64	1/2113 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	f	0.39	0/1434	0.66	0/1926
4	D	0.31	0/1665	0.52	0/2227
40	g	0.36	0/1343	0.59	1/1816 (0.1%)
41	h	0.27	0/1122	0.60	1/1515 (0.1%)
42	j	0.39	0/1152	0.63	0/1551
43	k	0.41	0/947	0.71	0/1268
44	l	0.41	0/1062	0.71	0/1413
45	m	0.41	0/1081	0.67	0/1443
46	n	0.42	0/973	0.71	0/1301
47	o	0.38	0/902	0.73	2/1209 (0.2%)
48	p	0.38	0/929	0.67	0/1242
49	q	0.45	0/960	0.74	0/1278
5	E	0.34	0/1118	0.56	0/1504
50	r	0.43	0/829	0.65	0/1107
51	s	0.39	0/864	0.70	0/1156
52	t	0.41	0/744	0.67	1/994 (0.1%)
53	u	0.39	0/787	0.68	0/1051
54	w	0.36	0/766	0.59	0/1025
55	y	0.38	0/576	0.64	0/762
56	z	0.46	1/215 (0.5%)	0.91	1/291 (0.3%)
6	F	0.28	0/835	0.53	0/1128
7	G	0.28	0/1187	0.51	0/1591
8	H	0.32	0/989	0.52	0/1326
9	I	0.31	0/1034	0.58	0/1375
All	All	0.50	88/158617 (0.1%)	0.87	466/237442 (0.2%)

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
27	2	0	1
34	b	0	64
35	c	0	1
37	d	0	1
43	k	0	1
44	l	0	1
50	r	0	1
9	I	0	1
All	All	0	71

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	2610	C	O3'-P	18.27	1.83	1.61
34	b	2123	G	C6-N1	17.59	1.51	1.39
34	b	2504	U	O3'-P	16.95	1.81	1.61
34	b	2123	G	N3-C4	16.78	1.47	1.35
34	b	2123	G	N9-C8	14.57	1.48	1.37

The worst 5 of 466 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	36	C	O3'-P-O5'	22.33	146.43	104.00
34	b	2602	A	P-O3'-C3'	15.43	138.22	119.70
34	b	1275	A	N9-C1'-C2'	15.08	133.61	114.00
34	b	1096	A	N9-C1'-C2'	-14.60	95.02	114.00
34	b	400	G	N9-C1'-C2'	14.53	132.89	114.00

There are no chirality outliers.

5 of 71 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	2	3	LYS	Peptide
9	I	124	PRO	Peptide
34	b	119	A	Sidechain
34	b	195	A	Sidechain
34	b	25	U	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32831	0	16518	776	0
2	B	1704	0	1732	54	0
3	C	1624	0	1699	62	0
4	D	1643	0	1710	92	0
5	E	1105	0	1148	43	0
6	F	817	0	808	29	0
7	G	1174	0	1230	37	0
8	H	979	0	1034	35	0
9	I	1022	0	1070	112	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	786	0	828	44	0
11	K	877	0	887	54	0
12	L	955	0	1019	30	0
13	M	876	0	936	39	0
14	N	774	0	827	38	0
15	O	716	0	742	21	0
16	P	649	0	664	121	0
17	Q	648	0	691	23	0
18	R	455	0	478	13	0
19	S	637	0	665	32	0
20	T	665	0	714	22	0
21	U	425	0	449	60	0
22	V	1620	0	817	145	0
23	W	1599	0	813	29	0
24	X	231	0	120	32	0
25	0	625	0	652	4	0
26	1	501	0	531	3	0
27	2	449	0	488	8	0
28	3	444	0	458	12	0
29	4	409	0	440	2	0
30	6	377	0	418	2	0
31	7	504	0	572	2	0
32	8	302	0	343	5	0
33	a	2506	0	1270	0	0
34	b	62321	0	31311	0	0
35	c	2082	0	2154	0	0
36	i	976	0	1008	0	0
37	d	1565	0	1616	0	0
38	e	1552	0	1619	0	0
39	f	1410	0	1444	0	0
40	g	1323	0	1371	0	0
41	h	1111	0	1148	0	0
42	j	1129	0	1162	0	0
43	k	938	0	1012	0	0
44	l	1053	0	1129	0	0
45	m	1063	0	1143	0	0
46	n	960	0	1000	0	0
47	o	892	0	923	0	0
48	p	917	0	961	0	0
49	q	947	0	1019	0	0
50	r	816	0	839	0	0
51	s	857	0	922	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	t	738	0	807	0	0
53	u	779	0	831	0	0
54	w	753	0	780	0	0
55	y	569	0	581	0	0
56	z	211	0	206	0	0
57	b	20	0	11	0	0
All	All	145911	0	97768	1662	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 1662 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:G:H21	16:P:13:LYS:NZ	1.05	1.47
21:U:27:VAL:O	21:U:31:VAL:CG1	1.65	1.43
1:A:392:C:C5'	16:P:12:LYS:HD2	1.47	1.41
1:A:375:U:H5'	16:P:6:LEU:CD2	1.50	1.39
9:I:112:ARG:NH2	9:I:114:LYS:HD2	1.39	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
2	B	216/241 (90%)	188 (87%)	19 (9%)	9 (4%)	3	25
3	C	204/233 (88%)	171 (84%)	23 (11%)	10 (5%)	3	20
4	D	203/206 (98%)	190 (94%)	9 (4%)	4 (2%)	9	43
5	E	148/167 (89%)	131 (88%)	7 (5%)	10 (7%)	1	12
6	F	98/131 (75%)	81 (83%)	14 (14%)	3 (3%)	5	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	148/156 (95%)	135 (91%)	8 (5%)	5 (3%)	5	30
8	H	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	12	48
9	I	125/130 (96%)	106 (85%)	16 (13%)	3 (2%)	7	38
10	J	96/103 (93%)	84 (88%)	7 (7%)	5 (5%)	2	19
11	K	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	21	61
12	L	121/124 (98%)	94 (78%)	22 (18%)	5 (4%)	3	25
13	M	111/118 (94%)	99 (89%)	5 (4%)	7 (6%)	2	14
14	N	92/101 (91%)	80 (87%)	8 (9%)	4 (4%)	3	24
15	O	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	16	54
16	P	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	3
17	Q	78/84 (93%)	66 (85%)	11 (14%)	1 (1%)	15	53
18	R	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	S	77/92 (84%)	69 (90%)	5 (6%)	3 (4%)	4	26
20	T	83/87 (95%)	77 (93%)	5 (6%)	1 (1%)	16	54
21	U	49/71 (69%)	40 (82%)	5 (10%)	4 (8%)	1	8
25	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
26	1	60/63 (95%)	53 (88%)	5 (8%)	2 (3%)	5	31
27	2	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	11	46
28	3	54/57 (95%)	49 (91%)	3 (6%)	2 (4%)	4	28
29	4	48/55 (87%)	39 (81%)	9 (19%)	0	100	100
30	6	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	3	22
31	7	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
35	c	269/273 (98%)	251 (93%)	17 (6%)	1 (0%)	39	76
36	i	132/142 (93%)	83 (63%)	38 (29%)	11 (8%)	1	8
37	d	207/209 (99%)	194 (94%)	11 (5%)	2 (1%)	19	59
38	e	199/201 (99%)	186 (94%)	7 (4%)	6 (3%)	5	34
39	f	175/179 (98%)	157 (90%)	12 (7%)	6 (3%)	5	30
40	g	174/177 (98%)	139 (80%)	31 (18%)	4 (2%)	8	40
41	h	147/149 (99%)	122 (83%)	20 (14%)	5 (3%)	5	30
42	j	140/142 (99%)	128 (91%)	10 (7%)	2 (1%)	14	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	k	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	11	47
44	l	142/144 (99%)	126 (89%)	10 (7%)	6 (4%)	3	25
45	m	131/136 (96%)	123 (94%)	7 (5%)	1 (1%)	24	63
46	n	118/127 (93%)	111 (94%)	4 (3%)	3 (2%)	7	38
47	o	114/117 (97%)	104 (91%)	5 (4%)	5 (4%)	3	23
48	p	112/115 (97%)	106 (95%)	5 (4%)	1 (1%)	21	61
49	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
50	r	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	34
51	s	108/110 (98%)	103 (95%)	2 (2%)	3 (3%)	6	35
52	t	91/100 (91%)	80 (88%)	8 (9%)	3 (3%)	5	31
53	u	100/104 (96%)	77 (77%)	12 (12%)	11 (11%)	0	3
54	w	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
55	y	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
56	z	25/27 (93%)	20 (80%)	5 (20%)	0	100	100
All	All	5630/5985 (94%)	5003 (89%)	458 (8%)	169 (3%)	9	34

5 of 169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	7	ASN
5	E	99	SER
8	H	44	PHE
9	I	57	VAL
12	L	88	ASP

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	
2	B	180/199 (90%)	180 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	113/126 (90%)	113 (100%)	0	100	100
6	F	87/112 (78%)	87 (100%)	0	100	100
7	G	123/129 (95%)	123 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	90/99 (91%)	90 (100%)	0	100	100
12	L	103/104 (99%)	103 (100%)	0	100	100
13	M	91/96 (95%)	91 (100%)	0	100	100
14	N	79/84 (94%)	79 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	57 (88%)	8 (12%)	6	25
17	Q	74/78 (95%)	74 (100%)	0	100	100
18	R	48/65 (74%)	48 (100%)	0	100	100
19	S	70/79 (89%)	70 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	44/61 (72%)	44 (100%)	0	100	100
25	0	67/68 (98%)	63 (94%)	4 (6%)	24	62
26	1	54/55 (98%)	52 (96%)	2 (4%)	41	75
27	2	48/49 (98%)	48 (100%)	0	100	100
28	3	47/48 (98%)	45 (96%)	2 (4%)	35	72
29	4	45/49 (92%)	45 (100%)	0	100	100
30	6	38/38 (100%)	37 (97%)	1 (3%)	54	82
31	7	51/52 (98%)	49 (96%)	2 (4%)	39	74
32	8	34/34 (100%)	33 (97%)	1 (3%)	50	80
35	c	216/218 (99%)	210 (97%)	6 (3%)	51	80
36	i	104/110 (94%)	87 (84%)	17 (16%)	3	13
37	d	164/164 (100%)	161 (98%)	3 (2%)	66	86
38	e	165/165 (100%)	159 (96%)	6 (4%)	42	76
39	f	148/150 (99%)	142 (96%)	6 (4%)	37	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	g	137/138 (99%)	133 (97%)	4 (3%)	50	80
41	h	114/114 (100%)	114 (100%)	0	100	100
42	j	116/116 (100%)	112 (97%)	4 (3%)	44	77
43	k	103/104 (99%)	101 (98%)	2 (2%)	65	85
44	l	103/103 (100%)	99 (96%)	4 (4%)	39	74
45	m	108/109 (99%)	107 (99%)	1 (1%)	84	93
46	n	100/103 (97%)	98 (98%)	2 (2%)	63	85
47	o	86/87 (99%)	86 (100%)	0	100	100
48	p	99/100 (99%)	95 (96%)	4 (4%)	38	74
49	q	89/90 (99%)	85 (96%)	4 (4%)	34	71
50	r	84/84 (100%)	80 (95%)	4 (5%)	31	69
51	s	93/93 (100%)	91 (98%)	2 (2%)	60	84
52	t	80/84 (95%)	77 (96%)	3 (4%)	40	75
53	u	83/85 (98%)	79 (95%)	4 (5%)	31	69
54	w	78/78 (100%)	76 (97%)	2 (3%)	54	82
55	y	56/63 (89%)	55 (98%)	1 (2%)	66	86
56	z	23/23 (100%)	13 (56%)	10 (44%)	0	0
All	All	4678/4879 (96%)	4569 (98%)	109 (2%)	61	83

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	e	93	SER
40	g	92	VAL
56	z	5	LYS
38	e	126	VAL
39	f	83	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	45	ASN
15	O	41	HIS
43	k	3	GLN
13	M	99	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	70	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1530/1542 (99%)	422 (27%)	30 (1%)
22	V	75/76 (98%)	45 (60%)	9 (12%)
23	W	75/75 (100%)	40 (53%)	10 (13%)
24	X	11/11 (100%)	8 (72%)	3 (27%)
33	a	116/120 (96%)	43 (37%)	0
34	b	2902/2904 (99%)	1204 (41%)	0
All	All	4709/4728 (99%)	1762 (37%)	52 (1%)

5 of 1762 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	22	G

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1157	A
1	A	1492	A
23	W	74	C
1	A	1201	A
1	A	1300	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
57	CLM	b	9000	-	18,20,20	0.74	0	23,27,27	0.83	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
57	CLM	b	9000	-	-	0/22/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	b	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	2610:C	O3'	2611:C	P	1.83
1	b	2504:U	O3'	2505:G	P	1.81
1	b	2248:C	O3'	2249:U	P	1.78
1	b	1323:C	O3'	1324:G	P	1.77