



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 31, 2017 – 11:49 AM EST

PDB ID : 3JBU
EMDB ID: : EMD-6483
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 : 3.64 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 : unknown
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

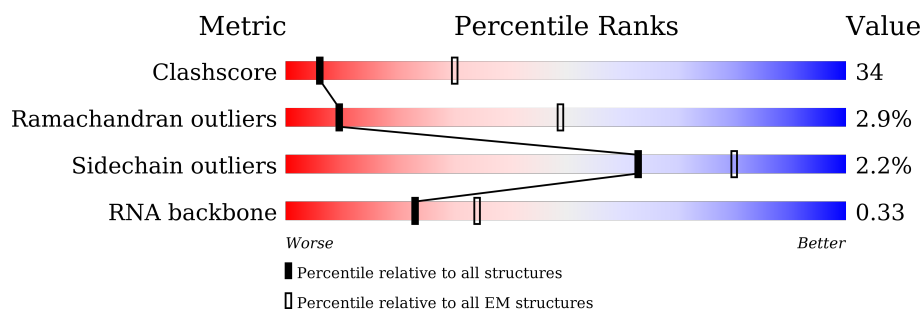
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 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.









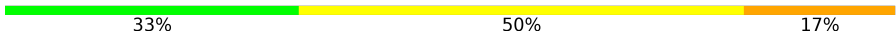

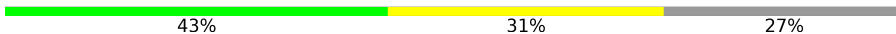
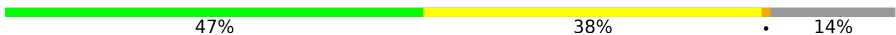

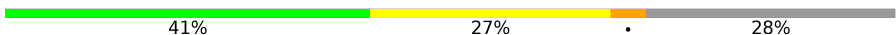








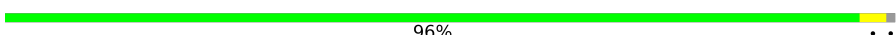
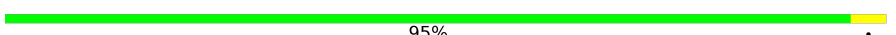
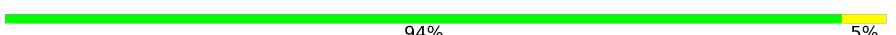

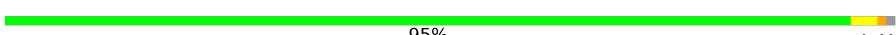
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	B	241	56% 32% • 10%
2	C	233	60% 27% • 12%
3	D	206	55% 43% •
4	E	167	58% 30% • 10%
5	F	131	42% 34% • 24%
6	G	156	67% 28% • •
7	H	130	66% 31% • •
8	I	130	50% 42% 5% •


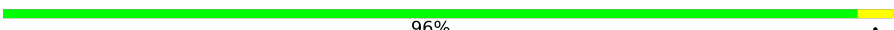
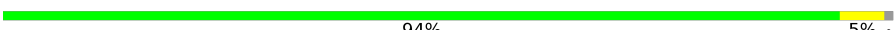
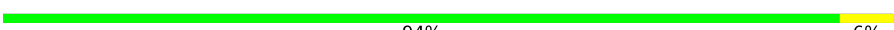
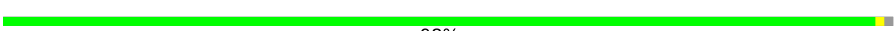





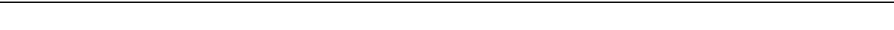

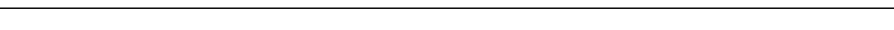
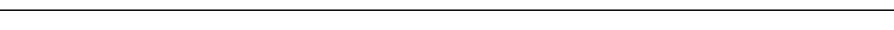
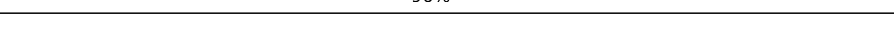






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Mol	Chain	Length	Quality of chain
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	U	71	
21	0	78	
22	1	63	
23	2	59	
24	3	57	
25	4	55	
26	6	46	
27	7	65	
28	8	38	
29	c	273	
30	d	209	
31	e	201	
32	f	179	
33	g	177	

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Mol	Chain	Length	Quality of chain
34	h	149	 90% 10%
35	j	142	 96% .
36	k	123	 94% 5% .
37	l	144	 94% 6%
38	m	136	 98% ..
39	n	127	 91% . . 6%
40	o	117	 92% 7% .
41	p	115	 95% . .
42	q	118	 97% ..
43	r	103	 94% 6%
44	s	110	 95% 5%
45	t	100	 89% . 7%
46	u	104	 89% 8% ..
47	w	94	 96% .
48	y	85	 88% 12%
49	z	87	 14% 16% 70%
50	A	1542	 36% 46% 17% .
51	X	11	 9% 27% 36% 27%
52	a	120	 62% 34% . .
53	b	2904	 55% 37% 6% .
54	v	76	 61% 39%

2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 143334 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 30S ribosomal protein S2.

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

- Molecule 2 is a protein called 30S ribosomal protein S3.

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

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

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

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

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

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	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 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

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

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

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

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S21.

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a protein called 50S ribosomal protein L4.

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

- Molecule 32 is a protein called 50S ribosomal protein L5.

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

- Molecule 33 is a protein called 50S ribosomal protein L6.

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

- Molecule 34 is a protein called 50S ribosomal protein L9.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called SecM-glycine.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	z	26	Total	C	N	O	0	0
			203	129	33	41		

- Molecule 50 is a RNA chain called 16S rRNA.

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

- Molecule 51 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	X	11	Total	C	N	O	P	0	0
			232	103	39	79	11		

- Molecule 52 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	118	Total	C	N	O	P	0	0
			2528	1126	464	821	117		

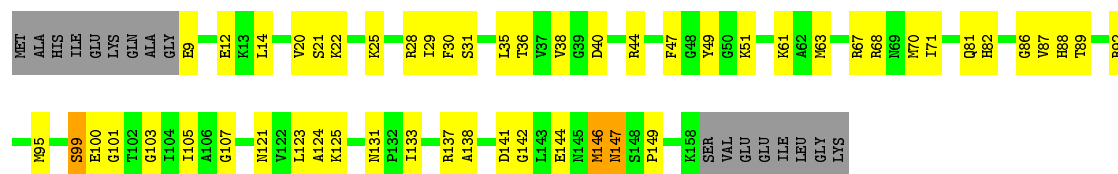
- Molecule 53 is a RNA chain called 23S rRNA.

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

- Molecule 54 is a RNA chain called glycine-tRNA.

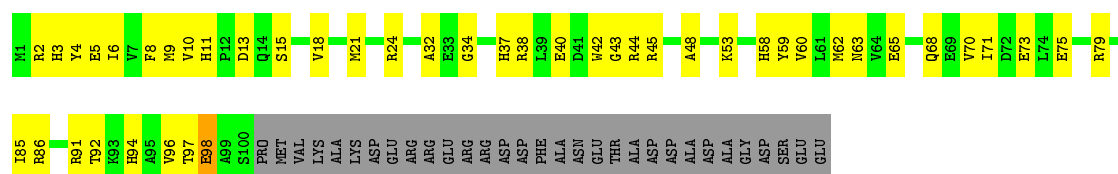
Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	76	Total	C	N	O	P	0	0
			1623	722	291	534	76		

Chain E:  58% 30% 10%



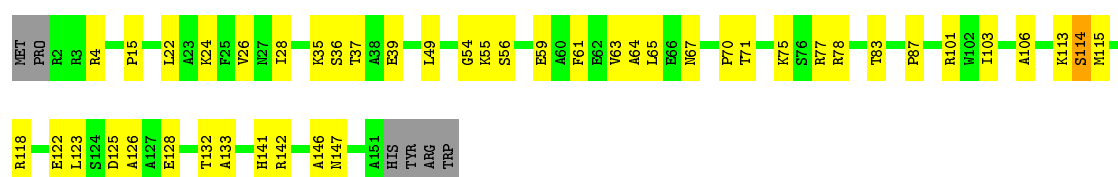
- Molecule 5: 30S ribosomal protein S6

Chain F:  42% 34% 24%



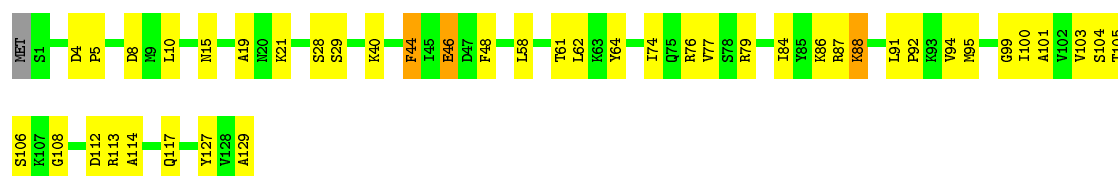
- Molecule 6: 30S ribosomal protein S7

Chain G:  67% 28% 2%



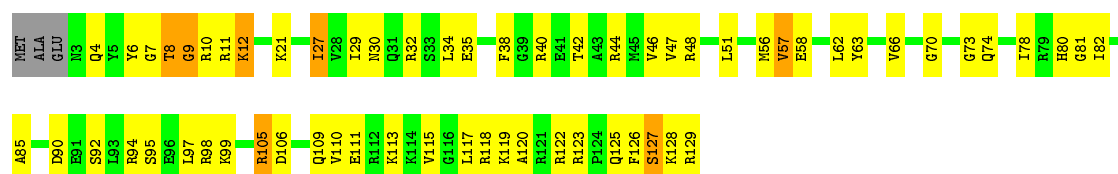
- Molecule 7: 30S ribosomal protein S8

Chain H:  66% 31% 2%



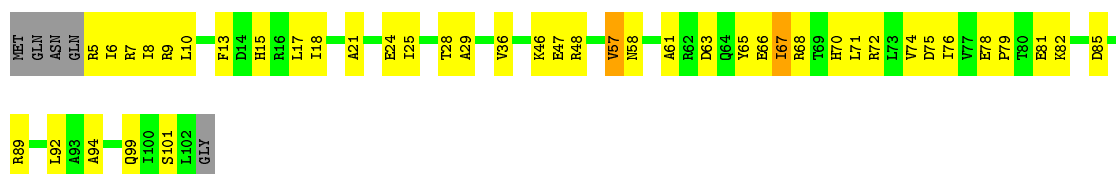
- Molecule 8: 30S ribosomal protein S9

Chain I:  50% 42% 5%



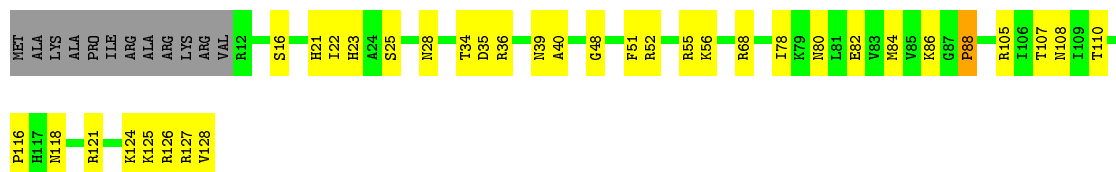
- Molecule 9: 30S ribosomal protein S10

Chain J:  53% 40% 5%



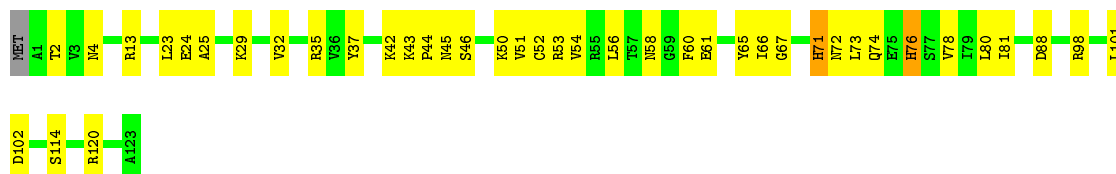
- Molecule 10: 30S ribosomal protein S11

Chain K: 64% 26% 9%



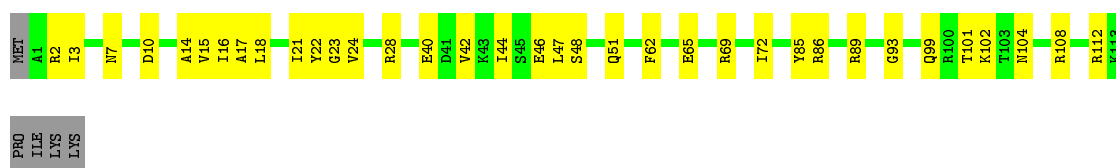
- Molecule 11: 30S ribosomal protein S12

Chain L: 66% 31% ..



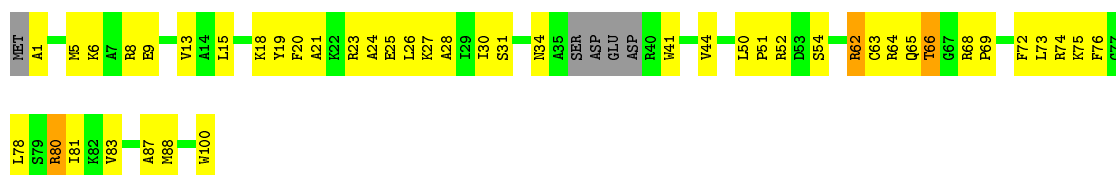
- Molecule 12: 30S ribosomal protein S13

Chain M: 66% 30% .



- Molecule 13: 30S ribosomal protein S14

Chain N: 50% 42% . 5%

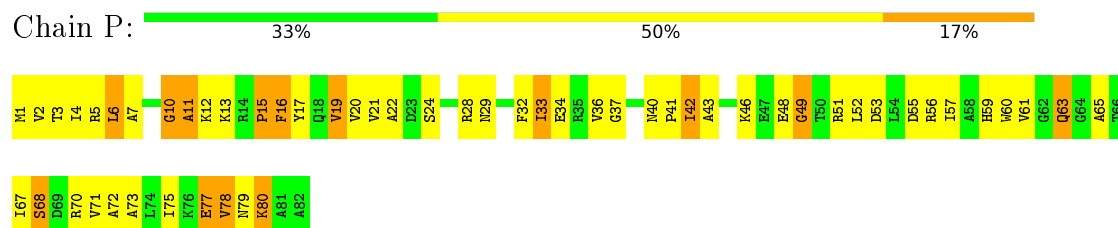


- Molecule 14: 30S ribosomal protein S15

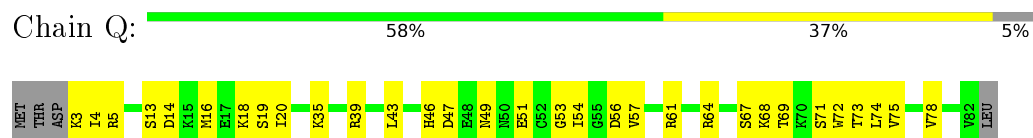
Chain O: 79% 18% ..



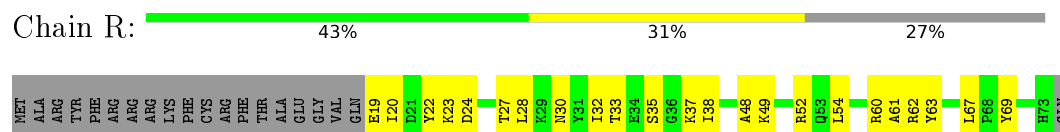
- Molecule 15: 30S ribosomal protein S16



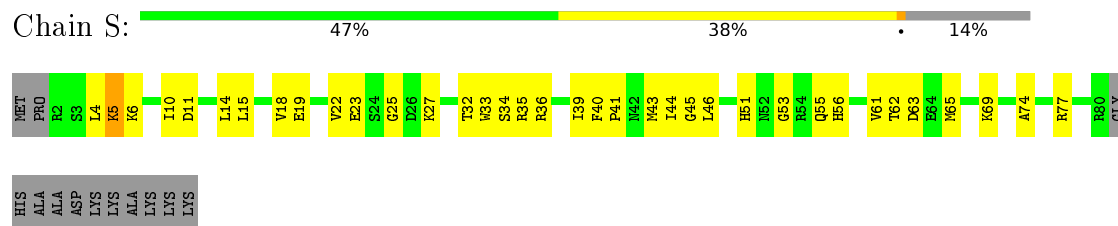
- Molecule 16: 30S ribosomal protein S17



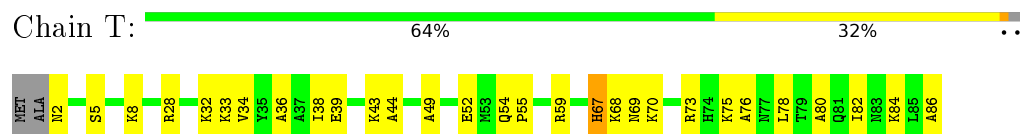
- Molecule 17: 30S ribosomal protein S18



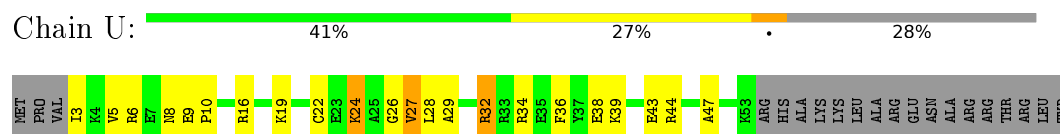
- Molecule 18: 30S ribosomal protein S19



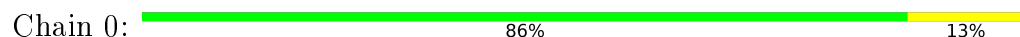
- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 50S ribosomal protein L28





- Molecule 22: 50S ribosomal protein L29

Chain 1: 78% 21% .



- Molecule 23: 50S ribosomal protein L30

Chain 2: 86% 8% . .



- Molecule 24: 50S ribosomal protein L32

Chain 3: 86% 12% .



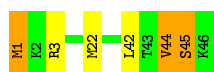
- Molecule 25: 50S ribosomal protein L33

Chain 4: 87% . 9%



- Molecule 26: 50S ribosomal protein L34

Chain 6: 87% 7% 7%



- Molecule 27: 50S ribosomal protein L35

Chain 7: 89% 9% .



- Molecule 28: 50S ribosomal protein L36

Chain 8: 82% 18%



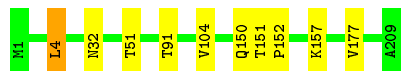
- Molecule 29: 50S ribosomal protein L2

Chain c:  96% ..



- Molecule 30: 50S ribosomal protein L3

Chain d:  95% .




- Molecule 31: 50S ribosomal protein L4

Chain e:  94% 5%



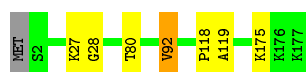
- Molecule 32: 50S ribosomal protein L5

Chain f:  92% 6% ..



- Molecule 33: 50S ribosomal protein L6

Chain g:  95% ..



- Molecule 34: 50S ribosomal protein L9

Chain h:  90% 10%



- Molecule 35: 50S ribosomal protein L13

Chain j:  96% .



- Molecule 36: 50S ribosomal protein L14

Chain k:  94% 5%



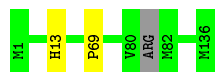
- Molecule 37: 50S ribosomal protein L15

Chain l:  94% 6%




- Molecule 38: 50S ribosomal protein L16

Chain m:  98% ..



- Molecule 39: 50S ribosomal protein L17

Chain n:  91% .. 6%



- Molecule 40: 50S ribosomal protein L18

Chain o:  92% 7%



- Molecule 41: 50S ribosomal protein L19

Chain p:  95% ..



- Molecule 42: 50S ribosomal protein L20

Chain q:  97% ..



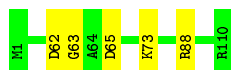
- Molecule 43: 50S ribosomal protein L21

Chain r:  94% 6%



- Molecule 44: 50S ribosomal protein L22

Chain s: 95% 5%



- Molecule 45: 50S ribosomal protein L23

Chain t: 89% 7%



- Molecule 46: 50S ribosomal protein L24

Chain u: 89% 8% ..



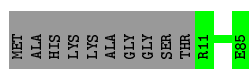
- Molecule 47: 50S ribosomal protein L25

Chain w: 96% .



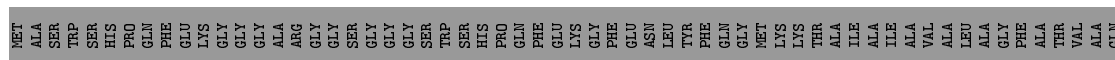
- Molecule 48: 50S ribosomal protein L27

Chain y: 88% 12%



- Molecule 49: SecM-glycine

Chain z: 14% 16% 70%

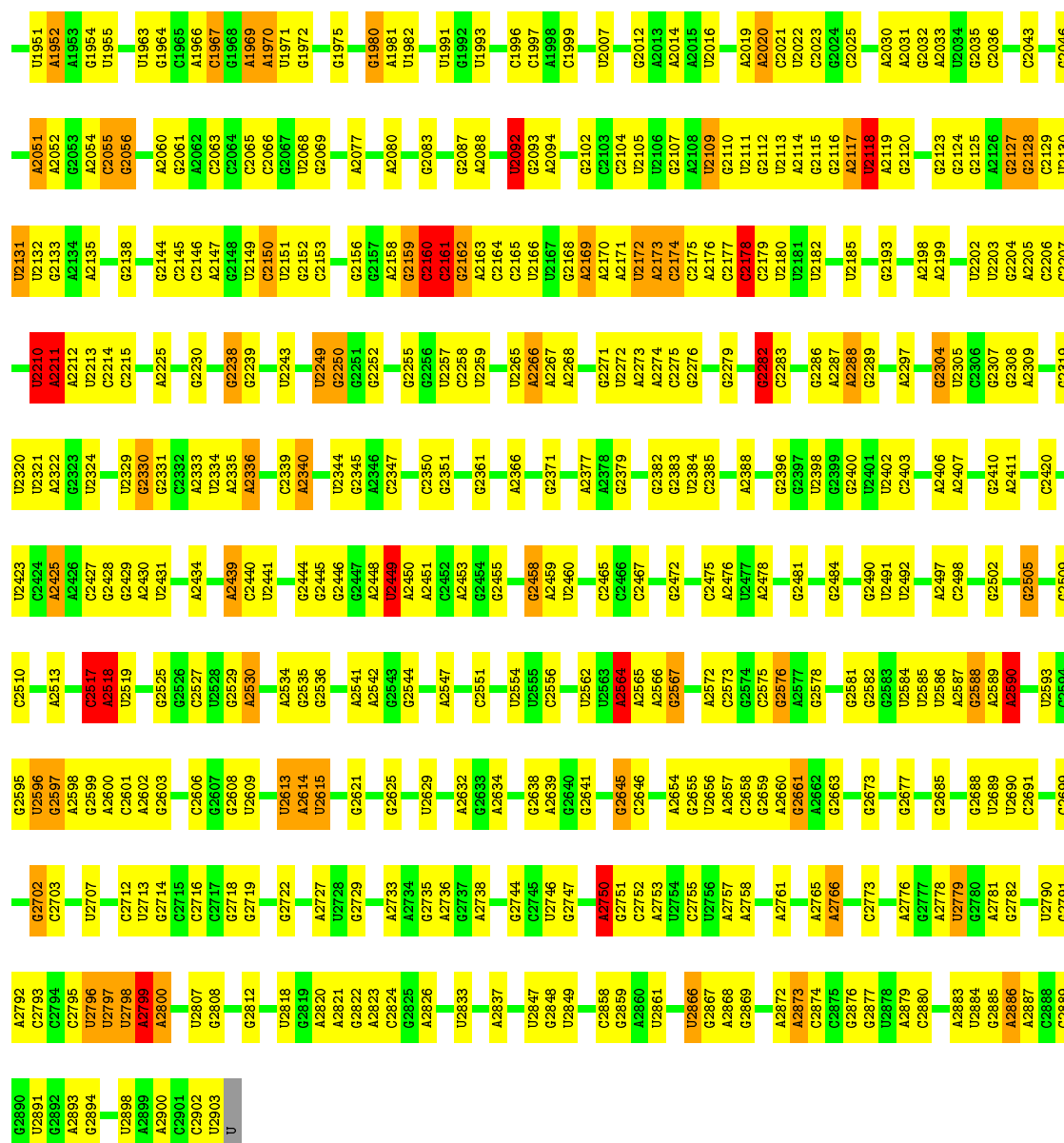


- Molecule 50: 16S rRNA

Chain A: 36% 46% 17% .

G1124	U1066	C990	C848	G771	A896	U619	G541	U473	G410	G347	U268	G201	C136	G64
U1125	G1057	U991	G849	U772	U697	C620	G542	G474	A411	G346	C272	G202	U137	A65
G1127	G993	U992	U850	G773	G698	A621	U543	U475	A412	A349	C277	G203	G138	C67
G1128	U1060	U994	G851	G779	G700	C623	C545	U477	A414	C352	G275	A205	U140	G68
G1129	G1061	C995	C853	U780	U701	C626	A546	A478	A415	A353	G276	U209	G143	G69
A1130	U1062	A996	C857	A781	A702	G627	A547	U479	G416	G354	C277	G210	G142	A7
G1131	C1063	U997	G858	A782	G703	G628	G548	U480	G417	C355	C278	G211	A143	A8
G1132	U1064	C998	G859	G786	A704	A629	C549	U481	C418	C356	A279	G212	G141	G11
G1133	U1065	C999	G860	A787	G705	A630	G550	A482	U420	G357	G278	G213	A74	G12
G1134	C1066	A1000	A860	G788	A706	A631	G551	C483	U421	G358	C279	G214	G140	G13
U1135	G1067	G1001	G861	U789	U707	C632	U552	G484	U422	G359	C280	G215	G146	G14
C1136	C1068	G1002	C864	U790	G708	G633	A553	U485	C423	G360	G281	G216	G147	U12
G1137	C1069	G1003	A864	A791	G709	C637	C556	U486	G424	G361	C282	G217	G148	U13
G1138	U1070	A1004	A865	G792	G710	U641	G557	U487	G425	G362	C283	G218	A149	U14
G1139	C1071	A1005	C866	A793	G711	A642	G558	A488	U426	A363	A288	U219	U150	G15
C1140	G1072	G1006	G869	U794	G712	G643	G559	C489	U427	A364	G289	U220	A151	A16
C1141	U1073	U1007	A870	A794	G713	G644	G560	U490	U428	U365	C290	G221	A152	U17
G1142	G1074	U1008	U871	G797	G714	G645	G561	C491	U429	U366	C291	G222	C153	C18
G1143	U1075	U1009	A872	C798	G715	G646	U562	C492	G430	U367	G292	U223	U154	A19
A1145	U1076	U1010	G873	U798	G716	C647	U563	G493	A431	U368	U296	G224	A155	U20
			U874	U801	G717	U648	U564	C494	A432	U369	C297	G225	C156	G21
			A875	A802	G718	U649	U565	G495	A433	C370	C300	A228	U157	G22
			G876	C806	G719	U650	G566	U496	U434	C371	A301	C229	A160	C23
			G877		G720	C651	G570	A497	A435	C372	G302	G230	A161	C25
			A878		G721	U652	U571	C498	C436	C373	C303	G231	A162	A26
			G879		G722	U653	U572	U499	U437	C374	G304	G232	C163	G27
			C882		G723	U657	G573	C503	C438	C375	U304	G233	C164	U28
					G724	U658	U574	C504	U439	C376	G305	G234	G165	U29
					G725	U659	G575	C505	C440	C377	A309	G235	U166	G31
					G726	U660	G576	C506	G441	C378	G310	A236	A167	U30
					G727	U661	G577	C507	G442	C379	C311	G239	C168	A32
					G728	U662	G578	C508	U443	C380	G312	U240	U170	A33
					G729	U663	U579	U509	G444	C381	C313	G241	C169	G34
					G730	U664	G580	C510	U445	C382	G314	G242	C170	G35
					G731	U665	G581	C511	G446	C383	U317	G243	A174	C36
					G732	U666	G582	U512	U447	C384	G318	U244	C175	G39
					G733	U667	G583	U513	G448	C385	C322	U245	C176	C40
					G734	U668	G584	C514	U449	C386	U323	A246	G177	G41
					G735	U669	G585	U515	G450	C387	G324	G247	C178	C42
					G736	U670	G586	U516	U451	C388	U325	U248	A181	C43
					G737	U671	G587	U517	A452	C389	A326	U249	A182	A44
					G738	U672	G588	C518	G453	C390	G327	A250	A183	G45
					G739	U673	G589	C519	U454	C391	C328	G251	C183	G46
					G740	U674	G590	C520	G455	C392	U329	U252	U184	C47
					G741	U675	G591	C521	U456	A393	C329	A253	U185	C48
					G742	U676	G592	C522	U457	C396	C330	G254	C186	
					G743	U677	G593	C523	U458	C397	G331	G255	A190	A51
					G744	U678	G594	C524	U459	U398	G332	G256	G191	C52
					G745	U679	G595	C525	U460	C400	C335	U257	G192	A53
					G746	U680	G596	C526	U461	C401	C336	G258	C193	C54
					G747	U681	G597	C527	U462	C402	C337	U259	G194	A55
					G748	U682	G598	C528	U463	C403	U338	G260	C195	U56
					G749	U683	G599	C529	U464	C404	G339	U261	A195	G128
					G750	U684	G600	C530	U465	C405	C340	G262	A196	G57
					G751	U685	G601	C531	U466	C406	U341	G263	A197	A60
					G752	U686	G602	C532	U467	C407	C342	G264	A198	G61
					G753	U687	G603	C533	U468	C408	U343	G265	G199	U62
					G754	U688	G604	C534	U469	C409	U344	G266	C200	C63
					G755	U689	G605	C535	U470	C410	U345	G267		
					G756	U690	G606	C536	U471	C411	U346	G268		
					G757	U691	G607	C537	U472	C412	U347	G269		
					G758	U692	G608	C538	U473	C413	U348	G270		
					G759	U693	G609	C539	U474	C414	U349	G271		
					G760	U694	G610	C540	U475	C415	U350	G272		
					G761	U695	G611	C541	U476	C416	U351	G273		
					G762	U696	G612	C542	U477	C417	U352	G274		
					G763	U697	G613	C543	U478	C418	U353	G275		
					G764	U698	G614	C544	U479	C419	U354	G276		
					G765	U699	G615	C545	U480	C420	U355	G277		
					G766	U700	G616	C546	U481	C421	U356	G278		
					G767	U701	G617	C547	U482	C422	U357	G279		
					G768	U702	G618	C548	U483	C423	U358	G280		
					G769	U703	G619	C549	U484	C424	U359	G281		
					G770	U704	G620	C550	U485	C425	U360	G282		
					G771	U705	G621	C551	U486	C426	U361	G283		
					G772	U706	G622	C552	U487	C427	U362	G284		
					G773	U707	G623	C553	U488	C428	U363	G285		
					G774	U708	G624	C554	U489	C429	U364	G286		
					G775	U709	G625	C555	U490	C430	U365	G287		
					G776	U710	G626	C556	U491	C431	U366	G288		
					G777	U711	G627	C557	U492	C432	U367	G289		
					G778	U712	G628	C558	U493	C433	U368	G290		
					G779	U713	G629	C559	U494	C434	U369	G291		
					G780	U714	G630	C560	U495	C435	U370	G292		
					G781	U715	G631	C561	U496	C436	U371	G293		
					G782	U716	G632	C562	U497	C437	U372	G294		
					G783	U717	G633	C563	U498	C438	U373	G295		
					G784	U718	G634	C564	U499	C439	U374	G296		
					G785	U719	G635	C565	U500	C440	U375	G297		
					G786	U720	G636	C566	U501	C441	U376	G298		
					G787	U721	G637	C567	U502	C442	U377	G299		
					G788	U722	G638	C568	U503	C443	U378	G300		
					G789	U723	G639	C569	U504	C444	U379	G301		
					G790	U724	G640	C570	U505	C445	U380	G302		
					G791	U725	G641	C571	U506	C446	U381	G303		
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					G800	U734	G650	C580	U515	C455	U390	G312		
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					G803	U737	G653	C583	U518	C458	U393	G315		
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					G805	U739	G655	C585	U520	C460	U395	G317		
					G806	U740	G656	C586	U521	C461	U396	G318		
					G807	U741	G657	C587	U522	C462	U397	G319		
					G808	U742	G658	C588	U523	C463	U398	G320		
					G809	U743	G659	C589	U524	C464	U399	G321		
					G810	U744	G660	C590	U525	C465	U400	G322		
					G811	U745	G661	C591	U526	C466</				

G1840	G1750	U1648	G1555	C1454	U1352	U1267	U1184	U1101	G1036	C951	G858	C758	U658	G570	C475
G1843	A1754	G1653	C1556	U1458	G1355	A1268	G1185	C1102	G1037	C951	G859	C763	G659	U571	C476
G1846	A1755	G1654	C1557	G1459	G1355	A1269	G1186	A1103	A1038	C957	A866	A764	G662	U572	A477
A1848	A1756	A1654	C1558	U1460	G1358	A1272	G1187	U1105	A1039	U958	C867	C765	G663	A574	A478
G1849	U1758	C1656	U1562	C1461	A1365	A1274	U1188	G1107	G1044	A960	U868	U766	G664	A575	A479
A1858	U1759	U1657	A1566	U1467	A1368	A1275	G1195	U1108	G1047	C961	G770	G770	A688	U576	A480
A1859	G1760	C1658	G1567	U1471	G1368	A1276	G1200	C1109	A1048	G962	U872	G775	G669	G583	A482
U1859	A1762	G1659	A1568	G1471	G1369	A1277	G1201	C1110	A1049	G963	C873	G776	A670	C584	A483
G1860	G1763	G1661	A1570	U1476	A1373	A1287	U1203	A1111	A1050	C964	G874	G777	C671	G585	G489
G1861	C1764	U1662	A1571	A1477	G1374	G1288	A1205	G1112	G1051	C965	G875	G777	G672	A586	C490
G1862	U1765	G1663	A1572	G1478	C1289	C1289	A1206	G1115	C1052	C968	C876	G778	G673	C587	G491
U1865	G1766	G1667	U1576	U1481	G1377	U1294	A1207	G1116	C1053	G969	A877	U779	G674	U588	A492
A1866	A1773	A1668	C1577	A1481	A1378	C1295	G1207	C1117	A1054	G972	A878	G780	A675	A603	G500
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C1868	U1775	G1674	A1583	G1483	G1382	G1299	U1209	G1122	A1057	A974	G882	G784	G696	U607	A502
G1869	G1776	C1675	U1584	U1487	A1383	G1300	G1210	G1125	U1058	G974	G785	G786	G701	A608	A503
A1870	A1780	A1678	C1585	A1494	A1384	A1301	G1211	A1126	G1059	A975	C787	G787	G612	A504	A505
A1871	A1781	G1679	A1592	A1495	U1390	A1302	G1218	U1130	U1061	A979	U887	G788	G704	A613	A508
G1873	A1783	G1681	U1593	A1496	U1391	A1306	G1221	U1131	G1062	A980	A789	A705	A704	A614	A509
A1880	A1784	G1682	C1595	U1497	A1392	A1307	U1222	G1133	C1063	A981	A790	U790	A706	U615	C509
G1887	A1785	U1683	G1598	C1498	A1393	G1223	G1223	U1132	C1064	C982	G791	G707	G616	A514	G510
U1897	A1786	G1687	A1598	C1499	U1394	G1311	U1224	A1133	U1066	A984	A792	G792	G711	G617	A514
C1905	A1787	G1687	U1599	G1500	A1395	U1312	G1225	A1134	G1067	C985	A793	A794	G712	G618	A518
G1905	G1792	G1687	A1600	A1503	U1396	U1313	G1226	G1136	A1069	A986	C997	G798	G713	A621	G519
G1906	C1793	U1693	G1601	G1507	U1397	U1314	G1227	G1137	A1070	G989	C988	G799	U714	G622	G520
G1907	A1794	C1694	G1602	C1508	U1400	U1316	U1231	G1138	G1071	C995	A899	A800	A715	G625	A526
C1908	A1800	G1695	A1603	A1509	U1401	U1318	G1232	G1139	C1072	A996	A900	C801	C717	A626	C527
A1913	A1801	G1697	C1606	G1510	U1402	C1319	U1234	U1141	A1073	G1003	C902	G805	C719	G628	A528
G1914	A1802	G1697	C1607	G1517	A1403	A1321	G1235	A1142	G1075	U1004	A910	G809	U720	A631	A529
U1915	A1803	G1699	A1608	G1522	G1408	A1322	G1236	A1143	C1076	C1005	A911	C812	A637	A632	G630
A1916	A1804	A1700	A1609	U1523	G1416	C1323	A1237	G1144	A1077	G1006	A912	A819	G636	A532	A538
U1917	G1807	G1703	C1610	A1524	G1416	U1326	G1238	G1145	C1078	A1010	A914	A822	U639	C640	C644
A1918	A1808	C1704	C1611	G1525	A1419	A1327	U1240	U1148	U1081	G1011	C915	A822	C640	U641	U545
A1919	A1809	A1706	A1616	G1526	A1420	U1328	G1241	A1156	A1084	U1012	A925	U827	U642	U546	A547
C1924	G1811	G1707	C1617	G1529	G1421	C1330	U1242	G1157	A1085	U1013	A925	U828	A643	A548	G549
A1927	G1814	G1710	A1618	G1530	G1422	G1332	U1249	G1163	A1086	U1018	A931	G830	G738	C645	C550
G1928	A1815	A1713	U1624	U1534	G1423	G1331	G1251	A1165	A1088	G1022	U932	G836	G745	U646	G559
G1929	G1816	U1714	G1624	G1425	G1425	G1337	G1253	A1169	A1089	U1023	U934	A844	U747	G651	C560
G1930	G1817	G1715	G1631	C1536	G1426	G1338	A1253	G1170	A1090	G1024	A941	U846	A750	U652	A563
U1931	G1817	G1715	G1632	G1537	G1428	G1341	U1254	C1171	G1091	G1025	A938	A845	A749	A654	C564
A1932	G1823	G1731	A1633	U1538	G1429	G1342	U1255	C1172	G1092	A1026	A941	U847	A751	A655	U568
A1936	G1824	C1732	G1634	U1539	G1435	G1343	G1256	U1173	U1094	A1027	A941	U847	A751	A655	U568
A1937	U1825	G1733	A1635	G1540	G1435	U1344	G1257	U1174	A1095	A1028	A941	U847	A751	A655	U568
A1938	G1826	G1733	G1635	C1541	U1438	G1259	U1260	U1175	A1096	A1032	A945	U847	A751	A655	U568
U1939	A1829	G1738	G1643	U1542	U1438	A1347	A1260	U1176	U1097	U1033	A945	U847	A751	A655	U568
U1940	U1940	A1739	C1644	U1542	U1438	A1347	A1260	U1176	U1097	U1033	A945	U847	A751	A655	U568
C1941	C1941	A1746	G1645	A1552	C1451	C1348	A1265	G1177	A1098	U1034	A945	U847	A751	A655	U568
U1943	U1943	A1746	U1647	U1554	A1453	C1349	A1266	G1178	A1099	U1035	A945	U847	A751	A655	U568
U1944	U1944	A1746	U1647	U1554	A1453	C1349	A1266	G1179	C1100	U1035	A945	U847	A751	A655	U568



• Molecule 54: glycine-tRNA

Chain v: 61% 39%



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 ⓘ

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	B	0.29	0/1735	0.51	0/2338
10	K	0.30	0/893	0.53	0/1205
11	L	0.36	0/969	0.59	0/1300
12	M	0.31	0/884	0.52	0/1181
13	N	0.34	0/785	0.54	0/1043
14	O	0.33	0/724	0.54	0/966
15	P	0.29	0/659	0.49	0/884
16	Q	0.34	0/657	0.53	0/881
17	R	0.37	0/462	0.58	0/621
18	S	0.32	0/652	0.55	0/877
19	T	0.33	0/671	0.52	0/888
2	C	0.33	0/1651	0.55	0/2225
20	U	0.33	0/430	0.63	0/570
21	0	0.38	0/635	0.67	0/848
22	1	0.37	0/502	0.65	0/667
23	2	0.39	0/453	0.61	0/605
24	3	0.41	0/450	0.73	0/599
25	4	0.38	0/416	0.58	0/554
26	6	0.44	0/380	0.77	0/498
27	7	0.37	0/513	0.62	0/676
28	8	0.38	0/303	0.74	0/397
29	c	0.39	0/2121	0.70	1/2852 (0.0%)
3	D	0.34	0/1665	0.55	0/2227
30	d	0.38	0/1586	0.63	1/2134 (0.0%)
31	e	0.39	0/1571	0.62	1/2113 (0.0%)
32	f	0.39	0/1434	0.66	0/1926
33	g	0.37	0/1343	0.56	0/1816
34	h	0.37	0/1122	0.68	5/1515 (0.3%)
35	j	0.37	0/1152	0.58	0/1551
36	k	0.38	0/947	0.68	1/1268 (0.1%)
37	l	0.38	0/1062	0.68	0/1413
38	m	0.38	0/1081	0.63	0/1443
39	n	0.39	0/973	0.67	0/1301
4	E	0.38	0/1118	0.56	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	o	0.39	0/902	0.70	0/1209
41	p	0.37	0/929	0.66	0/1242
42	q	0.39	0/960	0.69	1/1278 (0.1%)
43	r	0.40	0/829	0.67	1/1107 (0.1%)
44	s	0.35	0/864	0.67	1/1156 (0.1%)
45	t	0.40	0/744	0.66	1/994 (0.1%)
46	u	0.39	0/787	0.67	0/1051
47	w	0.36	0/766	0.58	0/1025
48	y	0.37	0/576	0.60	0/762
49	z	0.49	0/206	0.83	2/277 (0.7%)
5	F	0.32	0/835	0.56	0/1128
50	A	0.87	6/36762 (0.0%)	0.86	20/57350 (0.0%)
51	X	1.07	4/257 (1.6%)	0.91	0/396
52	a	0.45	1/2824 (0.0%)	0.93	7/4402 (0.2%)
53	b	0.55	52/69800 (0.1%)	1.03	441/108892 (0.4%)
54	v	0.36	1/1812 (0.1%)	0.85	4/2822 (0.1%)
6	G	0.31	0/1187	0.53	0/1591
7	H	0.35	0/989	0.55	0/1326
8	I	0.32	0/1034	0.61	0/1375
9	J	0.33	0/796	0.59	0/1077
All	All	0.60	64/155858 (0.0%)	0.89	487/233346 (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
11	L	0	1
23	2	0	1
29	c	0	1
30	d	0	1
36	k	0	1
37	l	0	1
43	r	0	1
52	a	0	1
53	b	0	72
All	All	0	80

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	A	230	G	C6-N1	60.83	1.82	1.39
50	A	230	G	N3-C4	58.56	1.76	1.35
50	A	230	G	C2-N3	55.19	1.76	1.32
50	A	230	G	N1-C2	53.83	1.80	1.37
50	A	230	G	C5-C4	53.10	1.75	1.38

The worst 5 of 487 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	A	230	G	N7-C8-N9	21.72	123.96	113.10
50	A	230	G	C2-N3-C4	19.69	121.75	111.90
50	A	230	G	N3-C4-N9	18.99	137.39	126.00
53	b	1509	A	N9-C1'-C2'	17.94	137.32	114.00
53	b	1275	A	N9-C1'-C2'	17.27	136.46	114.00

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	2	3	LYS	Peptide
11	L	71	HIS	Peptide
29	c	232	HIS	Peptide
30	d	151	THR	Peptide
36	k	34	GLY	Peptide

5.2 Too-close contacts [i](#)

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	B	1704	0	1732	61	0
2	C	1624	0	1699	49	0
3	D	1643	0	1710	83	0
4	E	1105	0	1148	44	0
5	F	817	0	808	32	0
6	G	1174	0	1230	29	0
7	H	979	0	1034	32	0
8	I	1022	0	1067	125	0
9	J	786	0	828	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	877	0	887	34	0
11	L	955	0	1019	35	0
12	M	876	0	935	27	0
13	N	774	0	827	39	0
14	O	716	0	742	14	0
15	P	649	0	663	119	0
16	Q	648	0	691	30	0
17	R	455	0	478	23	0
18	S	637	0	665	36	0
19	T	665	0	714	26	0
20	U	425	0	449	32	0
21	0	625	0	652	6	0
22	1	501	0	531	12	0
23	2	449	0	488	12	0
24	3	444	0	457	2	0
25	4	409	0	440	0	0
26	6	377	0	418	2	0
27	7	504	0	572	2	0
28	8	302	0	343	6	0
29	c	2082	0	2154	0	0
30	d	1565	0	1616	0	0
31	e	1552	0	1619	0	0
32	f	1410	0	1444	0	0
33	g	1323	0	1371	0	0
34	h	1111	0	1148	0	0
35	j	1129	0	1162	0	0
36	k	938	0	1012	0	0
37	l	1053	0	1129	0	0
38	m	1063	0	1143	0	0
39	n	960	0	1000	0	0
40	o	892	0	923	0	0
41	p	917	0	960	0	0
42	q	947	0	1019	0	0
43	r	816	0	839	0	0
44	s	857	0	922	0	0
45	t	738	0	807	0	0
46	u	779	0	831	0	0
47	w	753	0	780	0	0
48	y	569	0	581	0	0
49	z	203	0	198	0	0
50	A	32831	0	16518	889	0
51	X	232	0	118	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	a	2528	0	1283	0	0
53	b	62321	0	31336	0	0
54	v	1623	0	823	0	0
All	All	143334	0	95963	1594	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 34.

The worst 5 of 1594 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)
50:A:230:G:C6	50:A:230:G:C5	1.82	1.68
8:I:111:GLU:CB	50:A:1348:U:C4'	1.75	1.65
15:P:70:ARG:HG2	50:A:375:U:C5'	1.15	1.57
50:A:230:G:N3	50:A:230:G:C4	1.76	1.50
50:A:230:G:C5	50:A:230:G:C4	1.75	1.50

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	B	216/241 (90%)	186 (86%)	22 (10%)	8 (4%)	4	40
2	C	204/233 (88%)	173 (85%)	22 (11%)	9 (4%)	3	34
3	D	203/206 (98%)	179 (88%)	19 (9%)	5 (2%)	7	49
4	E	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	5	43
5	F	98/131 (75%)	82 (84%)	12 (12%)	4 (4%)	3	37
6	G	148/156 (95%)	128 (86%)	15 (10%)	5 (3%)	5	43
7	H	127/130 (98%)	111 (87%)	12 (9%)	4 (3%)	5	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	125/130 (96%)	99 (79%)	20 (16%)	6 (5%)	3	32
9	J	96/103 (93%)	77 (80%)	11 (12%)	8 (8%)	1	16
10	K	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	21	68
11	L	121/124 (98%)	100 (83%)	16 (13%)	5 (4%)	3	37
12	M	111/118 (94%)	100 (90%)	9 (8%)	2 (2%)	11	56
13	N	92/101 (91%)	78 (85%)	7 (8%)	7 (8%)	1	19
14	O	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	8	52
15	P	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	0	9
16	Q	78/84 (93%)	67 (86%)	9 (12%)	2 (3%)	7	48
17	R	53/75 (71%)	49 (92%)	4 (8%)	0	100	100
18	S	77/92 (84%)	66 (86%)	9 (12%)	2 (3%)	7	48
19	T	83/87 (95%)	78 (94%)	3 (4%)	2 (2%)	7	51
20	U	49/71 (69%)	39 (80%)	6 (12%)	4 (8%)	1	17
21	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
22	1	60/63 (95%)	51 (85%)	7 (12%)	2 (3%)	5	44
23	2	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	11	56
24	3	54/57 (95%)	49 (91%)	3 (6%)	2 (4%)	4	40
25	4	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
26	6	44/46 (96%)	41 (93%)	1 (2%)	2 (4%)	3	34
27	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
28	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
29	c	269/273 (98%)	252 (94%)	16 (6%)	1 (0%)	39	80
30	d	207/209 (99%)	195 (94%)	10 (5%)	2 (1%)	19	66
31	e	199/201 (99%)	186 (94%)	5 (2%)	8 (4%)	4	37
32	f	175/179 (98%)	154 (88%)	15 (9%)	6 (3%)	5	43
33	g	174/177 (98%)	139 (80%)	30 (17%)	5 (3%)	6	47
34	h	147/149 (99%)	120 (82%)	19 (13%)	8 (5%)	2	29
35	j	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	14	60
36	k	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	11	57
37	l	142/144 (99%)	128 (90%)	9 (6%)	5 (4%)	4	43
38	m	131/136 (96%)	125 (95%)	5 (4%)	1 (1%)	24	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	n	118/127 (93%)	111 (94%)	4 (3%)	3 (2%)	7	49
40	o	114/117 (97%)	107 (94%)	2 (2%)	5 (4%)	3	34
41	p	112/115 (97%)	106 (95%)	5 (4%)	1 (1%)	21	68
42	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
43	r	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	19	66
44	s	108/110 (98%)	103 (95%)	2 (2%)	3 (3%)	6	47
45	t	91/100 (91%)	82 (90%)	6 (7%)	3 (3%)	5	44
46	u	100/104 (96%)	82 (82%)	12 (12%)	6 (6%)	2	26
47	w	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
48	y	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
49	z	24/87 (28%)	21 (88%)	3 (12%)	0	100	100
All	All	5497/5903 (93%)	4898 (89%)	440 (8%)	159 (3%)	9	47

5 of 159 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	SER
2	C	7	ASN
2	C	61	LYS
4	E	99	SER
4	E	146	MET

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	B	180/199 (90%)	180 (100%)	0	100	100
2	C	170/190 (90%)	170 (100%)	0	100	100
3	D	172/173 (99%)	172 (100%)	0	100	100
4	E	113/126 (90%)	113 (100%)	0	100	100
5	F	87/112 (78%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	123/129 (95%)	123 (100%)	0	100	100
7	H	104/105 (99%)	104 (100%)	0	100	100
8	I	105/107 (98%)	104 (99%)	1 (1%)	82	92
9	J	86/90 (96%)	86 (100%)	0	100	100
10	K	90/99 (91%)	90 (100%)	0	100	100
11	L	103/104 (99%)	103 (100%)	0	100	100
12	M	91/96 (95%)	91 (100%)	0	100	100
13	N	79/84 (94%)	79 (100%)	0	100	100
14	O	76/77 (99%)	76 (100%)	0	100	100
15	P	65/65 (100%)	57 (88%)	8 (12%)	6	34
16	Q	74/78 (95%)	74 (100%)	0	100	100
17	R	48/65 (74%)	48 (100%)	0	100	100
18	S	70/79 (89%)	70 (100%)	0	100	100
19	T	65/66 (98%)	65 (100%)	0	100	100
20	U	44/61 (72%)	44 (100%)	0	100	100
21	0	67/68 (98%)	64 (96%)	3 (4%)	34	73
22	1	54/55 (98%)	52 (96%)	2 (4%)	41	77
23	2	48/49 (98%)	47 (98%)	1 (2%)	61	86
24	3	47/48 (98%)	46 (98%)	1 (2%)	61	86
25	4	45/49 (92%)	43 (96%)	2 (4%)	35	74
26	6	38/38 (100%)	35 (92%)	3 (8%)	15	55
27	7	51/52 (98%)	49 (96%)	2 (4%)	39	76
28	8	34/34 (100%)	34 (100%)	0	100	100
29	c	216/218 (99%)	210 (97%)	6 (3%)	51	82
30	d	164/164 (100%)	157 (96%)	7 (4%)	35	74
31	e	165/165 (100%)	158 (96%)	7 (4%)	36	75
32	f	148/150 (99%)	141 (95%)	7 (5%)	32	72
33	g	137/138 (99%)	134 (98%)	3 (2%)	60	85
34	h	114/114 (100%)	112 (98%)	2 (2%)	66	88
35	j	116/116 (100%)	113 (97%)	3 (3%)	54	83
36	k	103/104 (99%)	101 (98%)	2 (2%)	65	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	l	103/103 (100%)	100 (97%)	3 (3%)	50	81
38	m	108/109 (99%)	107 (99%)	1 (1%)	84	93
39	n	100/103 (97%)	97 (97%)	3 (3%)	48	81
40	o	86/87 (99%)	83 (96%)	3 (4%)	43	79
41	p	99/100 (99%)	95 (96%)	4 (4%)	38	76
42	q	89/90 (99%)	88 (99%)	1 (1%)	80	92
43	r	84/84 (100%)	81 (96%)	3 (4%)	42	78
44	s	93/93 (100%)	92 (99%)	1 (1%)	80	92
45	t	80/84 (95%)	80 (100%)	0	100	100
46	u	83/85 (98%)	79 (95%)	4 (5%)	31	72
47	w	78/78 (100%)	74 (95%)	4 (5%)	29	70
48	y	56/63 (89%)	56 (100%)	0	100	100
49	z	21/62 (34%)	9 (43%)	12 (57%)	0	0
All	All	4572/4808 (95%)	4473 (98%)	99 (2%)	63	85

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	f	7	TYR
35	j	30	THR
49	z	9	GLU
32	f	83	TYR
33	g	27	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
14	O	45	HIS
16	Q	44	HIS
44	s	7	HIS
14	O	50	HIS
15	P	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	A	1530/1542 (99%)	427 (27%)	36 (2%)
51	X	11/11 (100%)	7 (63%)	2 (18%)
52	a	116/120 (96%)	40 (34%)	0
53	b	2902/2904 (99%)	1211 (41%)	0
54	v	75/76 (98%)	27 (36%)	0
All	All	4634/4653 (99%)	1712 (36%)	38 (0%)

5 of 1712 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	A	6	G
50	A	7	A
50	A	8	A
50	A	9	G
50	A	11	G

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	A	702	A
50	A	997	U
50	A	1527	U
50	A	811	C
50	A	998	C

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	b	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	1087:G	O3'	1088:A	P	1.81
1	b	2055:C	O3'	2056:G	P	1.80