

SUPPLEMENTARY DATA

Automated 3D structure composition for large RNAs

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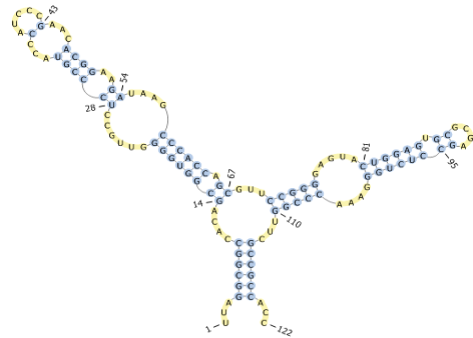
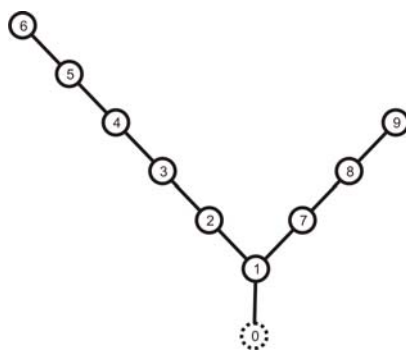
Supplementary Data are available at NAR online:

Supplementary tables S1-S9

Supplementary figures S1-S3

Supplementary dataset S1

TABLE S1. The RNA secondary structure fragmentation based on its tree graph representation. The 5S rRNA secondary structure as an example

 <p>5S rRNA <i>H. Marismortui</i> secondary structure derived from the X-ray structure (PDB ID 1FFK)</p>				 <p>5S rRNA tree graph representation (numbered)</p>				
Graph element	Structure element		Size [nt]	In-secondary structure localization		RNA FRABASE dictionary input pattern ^{a)}		
				first residue	last residue	strand name	secondary structure	
							sequence	topology
vertices								
0	single strands	5' end	4	1	4	strand1	^UUAG	^...()...\$
		3' end	4	119	122	strand2	CACC\$)...\$
1	3-way junction loop		16	9 67 110	14 71 114	strand1 strand2 strand3	CCACAG CGUUC GUUCG	(...()...()...)
2	bulge		5	15 64	16 66	strand1 strand2	CG CAG	(().)
3	internal loop		14	21 54	29 59	strand1 strand2	GGUUGCCU AUAAGC	(.....()....)
4	bulge		6	29 50	30 53	strand1 strand2	CC GAAG	(()..)
5	internal loop		10	33 43	37 47	strand1 strand2	UACCC GAACA	(...()....)
6	hairpin loop		7	37	43	strand1	CAUCCCG	(.....)
7	internal loop		13	75 101	81 106	strand1 strand2	GGAGUAC GGAAAC	(.....()....)
8	bulge		5	86 95	88 96	strand1 strand2	GUG CC	(.))
9	hairpin		6	89	94	strand1	CGCGAG	(.....)
edges								
1	stem		12	4 114	9 119	strand1 strand2	GGCGGC GCCGCC	((((())))))
2	stem		4	14 66	15 67	strand1 strand2	GC GC	(())
3	stem		12	16 59	21 64	strand1 strand2	GGUGGG CCCACC	((((())))))
4	stem		4	28 53	29 54	strand1 strand2	UC GA	(())
5	stem		8	30 47	33 50	strand1 strand2	CCGU ACGG	((()))
6	single base pair		2	37 43	37 43	strand1 strand2	C G	()
7	stem		10	71 106	75 110	strand1 strand2	CCGGG CCCGG	((((())))))
8	stem		12	81 96	86 101	strand1 strand2	CUGGAG CUCUGG	((((())))))
9	stem		4	88 94	89 95	strand1 strand2	GC GC	(())

^{a)} notation as reported in the RNA FRABASE (25)

TABLE S2. The RNA FRABASE dictionary statistics of secondary structure and tertiary structure elements

Structure element	Number of elements ^{a)}		
	secondary structure elements		tertiary structure elements
	sequence not specified	sequence specified	
Loops:			
hairpin	35	1,525	21,869
bulge and internal	338	5,458	70,604
3-way junction	889	1,874	13,740
4-way	928	1,422	8,584
5-way	720	910	6,580
6-way	174	210	1,164
7-way	336	392	1,680
8-way	112	128	200
9-way	27	27	27
10-way	40	50	50
11-way	217	230	231
12-way	48	58	60
14-way	14	14	14
Stems	17	1,828	63,417
Single strands:			
5'-end	10	38	155
3'-end	30	187	1,387
linking domains	21	113	1,166
All	3,956	14,464	190,928

^{a)} In order to increase the number of items in the dictionary, strand shift operation (25) was applied for such elements like bulges, internal and n-way junction loops.

TABLE S3. Statistical analysis of machine translation steps and properties of the 3D models predicted for a set of 95 RNAs with randomized sequence

No.	Strand length [nt]	Fragmentation number of secondary structure elements				In-dictionary search number of secondary structure elements			Refinement number of final 3D models			Secondary structure conservation [MCC] ^{a)}	Precision r.m.s.d. [Å] ^{b)}
		total	single strands	loops	stems	found with sequence similarity		missing	refined with energy		not refined		
						complete	not complete		low	high			
1	30	4	2	1	1	0	4	0	10	0	0	1.00	1.9
2	35	5	1	2	2	1	4	0	10	0	0	1.00	2.0
3	40	3	1	1	1	1	2	0	10	0	0	1.00	1.4
4	45	8	2	3	3	3	5	0	10	0	0	1.00	2.0
5	50	6	2	2	2	1	5	0	10	0	0	0.96	5.3
6	55	9	3	4	2	3	6	0	10	0	0	0.98	4.0
7	60	6	2	2	2	1	5	0	10	0	0	1.00	1.7
8	65	12	2	5	5	5	7	0	10	0	0	0.99	3.9
9	70	8	2	3	3	1	6	1	10	0	0	1.00	2.5
10	75	14	3	6	5	8	6	0	10	0	0	0.96	6.0
11	80	15	2	7	6	9	6	0	10	0	0	1.00	5.5
12	85	18	2	8	8	10	8	0	10	0	0	1.00	7.8
13	90	16	1	8	7	9	6	1	8	0	2	0.99	4.9
14	95	12	2	5	5	2	10	0	10	0	0	0.99	2.9
15	100	16	2	7	7	6	10	0	10	0	0	1.00	7.4
16	105	23	5	9	9	11	12	0	9	0	1	0.99	6.9
17	110	16	4	6	6	3	13	0	10	0	0	1.00	13.2
18	115	20	3	9	8	8	12	0	9	0	1	0.98	9.7
19	120	15	2	7	6	2	12	1	10	0	0	0.98	11.6
20	125	18	3	8	7	6	11	1	10	0	0	0.99	3.6
21	130	15	3	6	6	4	10	1	10	0	0	1.00	9.0
22	135	24	2	11	11	14	9	1	9	0	1	0.98	6.5
23	140	22	1	11	10	14	7	1	8	0	2	0.98	7.4
24	145	26	0	13	13	16	9	1	7	0	3	0.99	4.5
25	150	28	1	14	13	17	11	0	10	0	0	1.00	8.8
26	155	21	3	9	9	6	15	0	10	0	0	0.99	7.1
27	160	22	2	10	10	5	16	1	6	0	4	0.98	7.0
28	165	27	3	12	12	11	16	0	10	0	0	1.00	6.8
29	170	28	2	14	12	11	17	0	9	0	1	0.98	10.5
30	175	26	2	12	12	12	12	2	10	0	0	1.00	17.1
31	180	29	1	14	14	14	13	2	10	0	0	1.00	9.5
32	185	28	3	13	12	7	21	0	8	0	2	0.98	19.4
33	190	24	1	12	11	8	15	1	7	1	2	0.98	12.7
34	195	24	2	11	11	10	12	2	9	0	1	0.99	7.3
35	200	31	3	14	14	13	18	0	8	0	2	0.99	13.1
36	205	31	2	15	14	11	18	2	9	1	0	0.98	4.9
37	210	39	2	19	18	22	16	1	9	0	1	0.99	8.2
38	215	32	3	15	14	16	15	1	9	0	1	0.98	18.3
39	220	36	4	17	15	10	26	0	5	2	3	0.96	11.0
40	225	35	1	17	17	12	21	2	10	0	0	0.99	11.1
41	230	36	4	16	16	11	24	1	9	0	1	0.99	8.1
42	235	33	3	15	15	10	21	2	7	0	3	0.99	20.1
43	240	36	3	17	16	13	23	0	10	0	0	0.99	8.6
44	245	40	1	20	19	22	17	1	9	1	0	1.00	8.2
45	250	41	2	21	18	18	22	1	6	0	4	0.96	12.2
46	255	38	3	18	17	13	24	1	9	1	0	1.00	8.4
47	260	41	2	20	19	14	24	3	7	1	2	0.99	8.3
48	265	50	3	25	22	25	25	0	9	0	1	0.99	11.6
49	270	35	1	18	16	9	24	2	9	0	1	1.00	8.5
50	275	37	2	18	17	8	28	1	9	1	0	0.99	17.8
51	280	33	1	16	16	12	18	3	6	1	3	0.99	18.3
52	285	48	4	22	22	24	23	1	6	3	1	0.99	10.5
53	290	43	3	21	19	15	25	3	9	0	1	0.99	10.5
54	295	41	2	20	19	9	30	2	4	3	3	0.98	10.7
55	300	39	1	20	18	10	25	4	9	0	1	0.99	6.5
56	305	49	5	23	21	20	27	2	8	0	2	0.98	15.2
57	310	39	2	19	18	13	24	2	9	0	1	0.99	15.1
58	315	47	1	23	23	19	25	3	8	1	1	0.99	9.2
59	320	46	2	23	21	20	24	2	10	0	0	0.99	10.3
60	325	46	2	22	22	19	26	1	7	0	3	0.98	8.4
61	330	52	3	26	23	26	23	3	6	1	3	0.99	15.8
62	335	45	2	22	21	15	27	3	8	1	1	1.00	22.1

63	340	48	3	23	22	16	30	2	9	1	0	0.99	9.7
64	345	53	2	27	24	15	35	3	9	1	0	0.98	17.6
65	350	50	1	25	24	20	29	1	8	0	2	0.99	25.0
66	355	56	2	28	26	20	36	0	3	1	6	0.97	15.0
67	360	45	1	23	21	15	28	2	10	0	0	0.99	10.1
68	365	53	3	26	24	16	35	2	9	0	1	0.99	11.9
69	370	53	4	26	23	18	34	1	6	0	4	0.99	13.5
70	375	52	3	26	23	17	31	4	9	1	0	1.00	17.3
71	380	55	3	26	26	19	32	4	9	1	0	0.99	19.3
72	385	59	2	31	26	20	39	0	8	1	1	0.98	12.7
73	390	63	2	32	29	31	31	1	7	0	3	0.98	11.7
74	395	54	2	28	24	23	29	2	5	3	2	0.99	13.6
75	400	52	3	25	24	19	30	3	3	4	3	0.98	13.1
76	405	55	3	27	25	19	33	3	10	0	0	1.00	18.7
77	410	55	2	27	26	14	40	1	7	2	1	0.97	16.2
78	415	65	2	32	31	24	40	1	3	5	2	0.98	13.5
79	420	71	1	38	32	34	36	1	8	0	2	0.98	14.7
80	425	52	2	26	24	14	34	4	4	1	5	0.98	18.5
81	430	57	4	27	26	16	38	3	3	5	2	0.98	12.5
82	435	69	3	35	31	29	37	3	8	0	2	0.99	11.6
83	440	72	5	34	33	27	42	3	4	3	3	0.98	17.8
84	445	52	2	25	25	16	32	4	5	2	3	0.98	14.6
85	450	67	1	35	31	32	34	1	7	1	2	0.98	11.1
86	455	68	3	33	32	28	36	4	6	3	1	0.98	17.5
87	460	62	2	31	29	23	35	4	5	4	1	0.99	11.9
88	465	59	3	28	28	18	37	4	3	3	4	0.98	22.4
89	470	59	3	29	27	19	35	5	3	4	3	0.99	16.1
90	475	61	3	29	29	26	31	4	8	1	1	0.99	21.0
91	480	74	2	37	35	33	37	4	3	2	5	0.96	29.1
92	485	71	4	35	32	31	36	4	8	1	1	0.99	27.2
93	490	75	4	38	33	32	40	3	2	4	4	0.97	21.1
94	495	74	3	39	32	31	40	3	2	6	2	0.97	25.2
95	500	70	2	34	34	24	41	5	4	4	2	0.98	27.9
sum									741	82	127		

^{a)} Average of Matthews correlation coefficient (41) between the input and recovered secondary structures derived from the 10 final 3D models.

^{b)} Average heavy-atom r.m.s.d. between the 10 final RNA 3D models and their mean coordinates structure.

Table S4. 3D structure prediction details for the 500-mer RNA with randomized sequence

No.	Size [nt]	Target secondary structure element				Source tertiary structure element				Selection criteria					
		localization		secondary structure		localization		secondary structure		secondary structure topology ^{a)}	sequence similarity [%] ^{b)}	pyrimidines / purines compatibility [%] ^{c)}	source structure resolution [Å]	energy [kcal/mol]	
		residues				PDB ID	residues								
		first	last	sequence	topology		first	last	sequence						topology
Single strands															
0	5	1	5	GUACU(3I21 A	1	5	UGAAG(identical	20.0	20.0	3.7	-30.4
	6	495	500	AUUCAU).....	1F7U B	71	76	AAGCCA).....	identical	33.3	33.3	2.2	-47.6
Loops															
1	5	6	7	GA	((3I55 0	2279	2280	GA	((identical	100.0	100.0	3.1	-17.7
		492	494	UAC))		2290	2292	UAC))					
2	12	11	19	GACUAAUCU	(.....(1AUD B	18	26	CAUUGCACC	(.....(identical	33.3	58.3	- ^{d)}	-157.6
		486	488	GCC))		5	7	GAG))					
3	6	23	25	UAA	((1JZX A	1680	1682	UAA	((identical	100.0	100.0	3.1	-29.6
		480	482	UCA))		1978	1980	UCA))					
4	5	27	29	GUC	((1F7H A	5	7	GUC	((identical	100.0	100.0	- ^{d)}	-128.3
		477	478	GC))		22	23	GC))					
5	9	32	37	CGAAGC	(....(3E5C A	27	32	AGAUGC	(....(identical	66.7	66.7	2.2	-119.5
		472	474	GAG))		12	14	GAU))					
6	5	41	42	CC	((2ZJR X	863	864	CC	((identical	100.0	100.0	2.9	-75.9
		466	468	GCG))		938	940	GCG))					
7	8	47	48	CC	((1C2W B	2512	2513	CA	((identical	50.0	75.0	7.5	-105.2
		456	461	GAUACG))....)		2571	2576	UACGCG))....)					
8	12	55	58	UACU	((1NWX 0	2489	2492	CUCG	((identical	33.3	75.0	3.5	-174.1
		442	449	AACGUAGA)).....)		2550	2557	CACGCGAG)).....)					
9	6	60	62	UCU	((2GY9 A	80	82	UCU	((identical	83.3	100.0	15.0	-96.7
		438	440	AAA))		72	74	AGA))					
10	21	66	81	ACAUUAUGUAAACAG	(.....(missing in dictionary				tertiary structure element is generated					
		127	129	CAA))										
		433	434	UU))										
11	14	84	90	AAAAAAG	(.....(2AAR 0	2540	2546	AUUAAAG	(.....(identical	64.3	71.4	3.5	-113.0
		97	100	CCAC))		2496	2499	CAUC))					
		122	124	GCU))		2524	2526	GUU))					
12	6	91	96	GUCGUC	(....)	3JYX 5	1022	1027	GUCUUC	(....)	identical	83.3	83.3	8.9	-110.4
13	7	108	114	UCUCUUG	(.....)	2GYB A	803	809	UGUCUCG	(.....)	identical	71.4	85.7	15.0	-90.6
14	9	134	135	CG	((1NTB B	35	36	CG	((identical	77.8	77.8	2.9	-146.1
		422	428	CCUUUCG)).....)		7	13	CAUUUGG)).....)					
15	5	137	139	CAC	((1YL4 A	1242	1244	CAC	((identical	100.0	100.0	5.5	-91.0
		419	420	GG))		1255	1256	GG))					
16	6	143	144	AU	((1R2P A	8	9	AU	((identical	83.3	100.0	- ^{d)}	-70.2

17	9	412	415	AUGU)..)	24	27	ACGU)..)	identical	44.4	66.7	3.1	-55.7	
		146	147	GG	((2UUC A	738	739	CG	((
		154	156	CAG).(570	572	CGG).(
		407	410	UAAC)..)		635	638	CUAG)..)					
18	6	148	153	UUUAAG	(....)	3CMA 0	732	737	UUCAAG	(....)	identical	83.3	100.0	2.8	-54.6
19	19	163	164	GG	((missing in dictionary				tertiary structure element is generated					
		307	310	CAGU)..(
		388	400	AAAAACGGCAAGC).....)										
20	6	170	172	GCG	.(1U9S A	103	105	GCG	.(identical	100.0	100.0	2.9	-63.8
		299	301	CAC)..)		117	119	CAC)..)					
21	19	173	177	CGGCU	(...(missing in dictionary				tertiary structure element is generated					
		191	195	ACUGA)..(
		290	298	UAUAUUAAG).....)										
22	7	181	187	CCGUCUG	(.....)	3JYX 5	400	406	CCUUCGG	(.....)	identical	71.4	71.4	8.9	-77.1
23	8	198	201	UCUU	(.(3I8G 1	1755	1758	UUUU	(.(identical	87.5	100.0	3.1	-54.4
		284	287	AUCA)..)		1505	1508	AUCA)..)					
24	14	205	206	CG	((missing in dictionary				tertiary structure element is generated					
		269	280	UCCACCCAAAGG).....)										
25	12	210	215	CAUUUU	(....(2WR Q	1285	1290	CGGAUU	(....(identical	50.0	58.3	3.6	-4.3
		260	265	AUCCCG)....)	2WR A	1311	1316	AUGAAG)....)					
26	10	220	225	GGUCGU	(....(2OGO 0	1503	1508	GGUCAG	(....(identical	60.0	70.0	3.7	-94.3
		252	255	AAAC)..)		1514	1517	CUAC)..)					
27	5	227	229	ACG	.(1BVJ A	5	7	ACG	.(identical	100.0	100.0	- ^{d)}	-72.0
		249	250	CU)		18	19	CU)					
28	9	231	237	UUCUCUG	(.....(1NTA A	7	13	CAUUUGG	(.....(identical	33.3	77.8	2.9	-155.0
		246	247	CA)	1NTA B	35	36	CG)					
29	6	239	244	GCACAC	(....)	2WH4 A	681	686	GCACGC	(....)	identical	83.3	100.0	3.5	-47.8
30	22	313	325	GAACCUAAAUAAG	(.....(missing in dictionary				tertiary structure element is generated					
		364	365	CC)										
		379	385	GAAACCC).....)										
31	6	328	330	UAA	.(2QBA B	2446	2448	CAA	.(identical	83.3	100.0	3.5	-43.9
		359	361	UAG)..)		2507	2509	UAG)..)					
32	16	332	339	AGUUCUAC	(.....(2VHP A	673	680	AGAAUUC	(.....(identical	56.2	68.8	3.7	-151.5
		350	357	GGCACA AU).....)		710	717	GGAGGA AU).....)					
33	10	340	349	CGAGACUAAG	(.....)	1P9X 0	2383	2392	CGUGUGGAAG	(.....)	identical	60.0	60.0	3.4	-99.2
34	7	369	375	GUAGCGC	(.....)	1U9S A	10	16	GUAACGC	(.....)	identical	85.7	100.0	2.9	-58.3
Stems															
1	4	5	6	UG	((3MS0 A	894	895	UG	((identical	100.0	100.0	3.6	-38.4
		494	495	CA)		1373	1374	CA)					
2	10	7	11	AGCGG	(((((2VHM B	1396	1400	AGCGG	(((((identical	100.0	100.0	3.7	-206.3
		488	492	CCGCU))))		1410	1414	CCGCU))))					
3	10	19	23	UGUAU	(((((3CF5 X	835	839	UGUAU	(((((identical	80.0	100.0	3.3	-178.4
		482	486	AUACG))))		844	848	GUACA))))					
4	6	25	27	AUG	((1VOZ A	595	597	AUG	((identical	100.0	100.0	11.5	-93.9
		478	480	CGU)		627	629	CGU)					
5	8	29	32	CGAC	(((((1J5A A	1178	1181	CAAC	(((((identical	87.5	100.0	3.5	-144.3
		474	477	GUUG))))		1193	1196	GUUG))))					

6	10	37 41 CCGGC 468 472 GCCGG	((())))	1P9X 0	589 593 CCGGC 1269 1273 GCCGG	((())))	identical	100.0	100.0	3.4	-104.8
7	12	42 47 CUUCGC 461 466 GCGAAG	((())))	1QVF 0	930 935 CUCCGC 1033 1038 GCGGGG	((())))	identical	75.0	100.0	3.1	-111.2
8	16	48 55 CGUUAACU 449 456 AGUUAACG	((((())))))	3E1B B	268 275 CAUUAACU 285 292 GGUUA AUG	((((())))))	identical	81.2	100.0	9.0	-227.7
9	6	58 60 UCU 440 442 AGA	(())	2FRL A	7 9 UCU 15 17 AGA	(())	identical	100.0	100.0	- ^{d)}	-100.0
10	10	62 66 UCAUA 434 438 UGUGA	((())))	2OGO 0	2827 2831 GCAUA 2836 2840 UGUGU	((())))	identical	80.0	80.0	3.7	-12.8
11	8	81 84 GGAA 124 127 UUCC	((())))	1W2B 0	1408 1411 GGAU 1696 1699 GUCC	((())))	identical	75.0	75.0	3.5	-118.2
12	4	90 91 GG 96 97 CC	(())	3BBX B	1593 1594 GG 1600 1601 CC	(())	identical	100.0	100.0	10.0	-69.9
13	18	100 108 CUGAGUGCU 114 122 GGUUAUCAG	((((())))))	1YJ9 0	2381 2389 CAGUGUUCU 2399 2407 GGAACGCUG	((((())))))	identical	61.1	66.7	2.9	-340.3
14	12	129 134 AGUGGC 428 433 GCCAUU	((())))	3CUL C	2 7 GAUGGC 12 17 GCCAUU	((())))	identical	83.3	100.0	2.8	-93.7
15	6	135 137 GGC 420 422 GCC	(())	1HNX A	489 491 GGC 508 510 GCC	(())	identical	100.0	100.0	3.4	-117.6
16	10	139 143 CCGUA 415 419 UACGG	((())))	1JGQ D	178 182 CCGGA 190 194 UCCGG	((())))	identical	80.0	80.0	5.0	-188.5
17	6	144 146 UCG 410 412 CGA	((())))	3EPJ F	71 73 UCG 135 137 CGA	((())))	identical	100.0	100.0	3.1	-58.3
18	4	147 148 GU 153 154 GC	(())	1PNY 0	1865 1866 GU 1871 1872 GC	(())	identical	100.0	100.0	9.5	-97.6
19	16	156 163 GAUAGACG 400 407 CGUCUAUU	((((())))))	1VS6 B	1284 1291 CAGCGACG 1298 1305 CGUUGUUG	((((())))))	identical	56.2	62.5	3.5	-270.5
20	14	164 170 GAAGGAG 301 307 CUCCUUC	((())))	3JYV A	1432 1438 GACGGAG 1485 1491 CUCCGUC	((())))	identical	85.7	85.7	8.9	-298.8
21	4	172 173 GC 298 299 GC	(())	3D5B A	1116 1117 GC 1124 1125 GC	(())	identical	100.0	100.0	3.2	-103.0
22	10	177 181 UGCGC 187 191 GCGUA	((())))	2HEM A	6 10 GCGCG 15 19 GCGUC	((())))	identical	80.0	80.0	- ^{d)}	-259.9
23	8	195 198 AUAU 287 290 AUGU	((())))	2BYT E	110 113 GCAU 125 128 AUGU	((())))	identical	75.0	100.0	3.3	-104.9
24	10	201 205 UCUC 280 284 GGAGA	((())))	1YL3 A	2595 2599 UCUC 2621 2625 GGAGG	((())))	identical	90.0	100.0	5.5	-160.3
25	10	206 210 GGAGC 265 269 GCUCU	((())))	3BBO A	2647 2651 AGAGC 2802 2806 GCUCU	((())))	identical	90.0	100.0	9.4	-183.4
26	12	215 220 UGUAGG 255 260 CCUAUA	((())))	3A3A A	28 33 UGCAGG 41 46 CCUGUA	((())))	identical	83.3	100.0	3.1	-159.9
27	6	225 227 UGA 250 252 UCA	(())	3CCU 0	560 562 UGA 595 597 UCA	(())	identical	100.0	100.0	2.8	-69.2
28	6	229 231 GCU 247 249 AGC	((())))	2WRR A	325 327 GCU 338 340 AGC	((())))	identical	100.0	100.0	3.6	-34.5
29	6	237 239 GAG	(((1PNX A	402 404 GAG	(((identical	100.0	100.0	9.5	-89.8

		244	246	CUC)))		428	430	CUC)))					
30	8	310	313	UCGG	(((2QBG B	992	995	UCGG	(((identical	100.0	100.0	3.3	-96.7
		385	388	CCGA))))		1022	1025	CCGA))))					
31	8	325	328	GUAU	(((2QAL A	406	409	GUAU	(((identical	100.0	100.0	3.2	-69.9
		361	364	GUAC))))		433	436	GUAC))))					
32	6	330	332	ACA	(((1JGO D	162	164	ACA	(((identical	100.0	100.0	5.6	-108.5
		357	359	UGU)))		174	176	UGU)))					
33	4	339	340	CC	((3MRZ A	1026	1027	CC	((identical	100.0	100.0	3.6	-73.4
		349	350	GG)		1155	1156	GG)					
34	10	365	369	CGUUG	(((2QAO B	2935	2939	CGUUG	(((identical	90.0	100.0	3.2	-178.4
		375	379	CAACG))))		2947	2951	CGACG))))					

a) encompassing the secondary structure element size, number and length of RNA strands

b) between the target and source RNA sequence

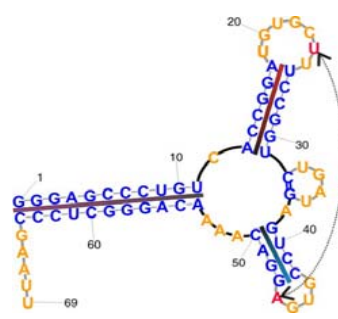

c) shows matching of the purine / pyrimidine residues for the target and source RNA of given sequence

d) the NMR structure as a source

Table S5. MolProbity RNA structure stereochemical quality assessment for the 3D models predicted by RNAComposer for set of 40 benchmark structures described in the Table 1. An assessment includes respective high-resolution X-ray structures.

PDB code and chain	RNA strand length [nt]	clash-score, all atoms		nucleic acid geometry							
				potentially incorrect				outlier bonds [%]		outlier angles [%]	
		sugar puckers		backbone conformations							
		RNA Composer	X-ray	RNA Composer	X-ray	RNA Composer	X-ray	RNA Composer	X-ray	RNA Composer	X-ray
<i>hairpin</i>											
2DR8 B	33	17.92	33.87	1	3	7	6	0.00	0.00	0.00	0.00
3OVA C	34	16.64	6.45	2	2	6	3	0.00	0.00	0.00	17.65
<i>hairpin internal loop</i>											
1JBR D	31	16.93	6.95	0	1	3	7	0.00	6.45	0.00	3.23
2HW8 B	36	12.90	4.28	1	1	3	4	0.00	0.00	0.00	11.11
1ZHO B	38	12.23	12.21	1	1	5	3	0.00	2.63	0.00	13.16
3IAB R	46	16.90	13.50	2	3	11	12	0.00	2.17	0.00	17.39
<i>hairpin internal loops</i>											
116U C	37	14.31	9.20	1	4	4	7	0.00	0.00	0.00	8.11
2PXL B	47	15.79	11.47	0	0	5	1	0.00	0.00	0.00	0.00
2VPL B	48	12.24	3.22	2	3	10	8	0.00	0.00	0.00	27.08
2PXB B	49	11.46	11.58	0	0	5	2	0.00	0.00	0.00	0.00
1MZP B	55	13.48	14.00	4	7	10	9	0.00	0.00	0.00	7.27
1KXX A	70	19.07	27.47	1	4	16	15	0.00	0.00	0.00	1.43
<i>three-way junction</i>											
1DK1 B	57	19.57	37.28	3	3	9	13	0.00	3.51	0.00	8.77
1MMS C	58	15.56	14.41	0	0	7	3	0.00	0.00	0.00	0.00
1UN6 E	61	14.23	26.40	1	0	9	6	0.00	0.00	0.00	0.00
<i>three-way junction (hammerhead)</i>											
2QUS A	69	12.63	8.5	0	5	11	19	0.00	1.47	0.00	41.18
<i>three-way junction (riboswitch)</i>											
3LA5 A	71	18.57	6.13	1	2	8	1	0.00	0.00	0.00	7.04
3D2V A	77	18.51	11.03	1	1	11	10	0.00	0.00	0.00	2.60
<i>three-way junction (GMP riboswitch)</i>											
3IWN A	93	7.99	38.36	0	11	13	25	0.00	0.00	0.00	10.75
<i>three-way junction (SRP)</i>											
2V3C M	96	17.70	65.64	2	16	19	52	0.00	56.25	0.00	98.96
1LNG B	97	15.95	41.76	1	10	26	39	0.00	6.19	0.00	49.48
1Z43 A	101	14.38	76.81	1	14	25	54	0.00	35.64	0.00	87.13
3NDB M	136	13.87	31.14	2	14	28	68	0.00	8.09	0.00	74.26
<i>three-way junction (5S rRNA)</i>											
3OFQ B	117	17.48	64.06	2	16	24	44	0.00	0.00	0.00	22.22
3OFR B	118	14.44	33.82	3	17	19	34	0.00	0.00	0.00	36.44
3KIR B	119	15.56	22.34	1	1	23	18	0.00	0.00	0.00	0.84
3I9E B	120	13.92	35.83	0	6	18	21	0.00	0.00	0.00	5.00
1VQO 9	122	14.01	15.01	1	2	24	16	0.00	0.00	0.00	0.82
<i>four-way junction (tRNA)</i>											
1EXD B	73	8.10	46.77	2	12	16	19	0.00	0.00	0.00	12.33
1U0B A	74	16.44	22.74	7	8	15	15	0.00	1.35	0.00	1.35
1FFY T	75	19.47	26.39	6	12	18	25	0.00	0.00	0.00	5.33
2J00 W	76	18.44	40.92	2	3	18	15	0.00	0.00	0.00	6.58
<i>four-way junction (riboswitch)</i>											
3IQP A	94	13.12	35.29	5	10	17	27	0.00	2.13	0.00	11.70
<i>five-way junction (tRNA)</i>											
3AM1 B	81	16.08	42.46	4	6	14	22	0.00	0.00	0.00	30.86
1WZ2 C	88	13.06	32.09	4	7	26	24	0.00	0.00	0.00	6.82
3ADB C	92	17.18	21.20	1	1	16	13	0.00	1.09	0.00	4.35
<i>pseudoknot</i>											
2QWY A	52	22.67	39.77	2	3	13	15	0.00	0.00	0.00	1.92
<i>pseudoknot (HDV ribozyme)</i>											
1CX0 B	72	12.96	24.09	3	8	16	16	0.00	0.00	0.00	9.72
<i>P4-P6 ribozyme domain</i>											
2R8S R	159	12.89	2.34	10	5	21	14	10.06	0.00	10.06	8.81
<i>M-box riboswitch</i>											
3PDR A	161	17.83	8.11	1	2	30	17	0.00	0.00	0.00	11.80
average		15.31	25.62	2.03	5.60	14.47	18.05	0.25	3.17	0.25	16.59

Table S6. RNA 3D structure prediction details for the n-way junctions

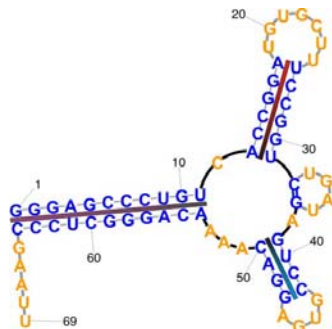
PDB code 2QUS; three-way junction (hammerhead)										Input data					
GGGAGCCCUGUCACCGGAUGUGCUUCCGGUCUGAUGAGUCGUGAGGACAAAACAGGGCUCCGAAUU										Secondary structure derived from the RNA FRABASE					
(((((((((((.((((.....[.]))))))).....).(((...])))).....)))))).....										Note the square bracket for U24-A46 loop-loop interaction					
						Model No.			Energy [kcal/mol]		r.m.s.d. [Å]				
Secondary structure visualization			10 superimposed 3D models			1		-1622		3.7					
						2		-1637		3.4					
						3		-1585		3.8					
						4		-1598		3.7					
						5		-1555		4.3					
						6		-1622		3.6					
						7		-1584		3.8					
						8		-1620		4.1					
						9		-1601		3.8					
						10		-1580		3.9					
Lowest r.m.s.d. 3D model (No. 2)															
Details of the model No. 2 prediction ^{a)}															
No.	Size [nt]	Target secondary structure element				Source tertiary structure element				Selection criteria					
		localization		secondary structure		localization		secondary structure		secondary structure topology ^{b)}	sequence similarity [%] ^{c)}	pyrimidines / purines compatibility [%] ^{d)}	source structure resolution [Å]	energy [kcal/mol]	
		residues		sequence	topology	PDB ID	residues		sequence						topology
		first	last				first	last							
Single strands															
0	6	64	69	CGAAUU).....	2QUW D	133	138	CGAAUU).....	identical	100.0	100.0	2.2	-78.8
Loops															
1	13	11	13	UCA	((2GOZ B	48	50	UCC	((identical	76.9	84.6	2.2	-267.9
		31	32	UC)	2GOZ A	14	15	GC)					
		37	39	GAG).		20	22	GAG).					
		50	54	CAAAA	...)		35	39	CGAAA	...)					
2	9	18	26	AUGUGCUUU	(.....[.)	2QUW B	18	26	AUGUGCUUU	(.....[.)	identical	100.0	100.0	2.2	-98.7
3	6	32	37	CUGAUG	(.....)	2GOZ A	15	20	CUGAUG	(.....)	identical	100.0	100.0	2.2	-127.2
4	6	42	47	CGUGAG	(...)	2QUW D	111	116	CGUGAG	(...)	identical	100.0	100.0	2.2	-87.4
Stems															
1	22	1	11	GGGAGCCCUGU	((((((((2HGQ A	15	25	GGGCCACGGU	((((((((identical	54.5	63.6	5.5	-493.5
		54	64	ACAGGGCUCCC)))))))))		541	551	ACCGUGGGCUU)))))))))					
2	12	13	18	ACCGGA	(((2G5K A	10	15	UCCGGA	(((identical	83.3	83.3	2.8	-200.6
		26	31	UCCGGU))))	2G5K B	33	38	UCCGGA))))					
3	2	32	32	C	(single base pair - not used					single base pair - not used				
		37	37	G)										
4	8	39	42	GUCC	(((2GOZ A	22	25	GUCC	(((identical	100.0	100.0	2.2	-171.5
		47	50	GGAC)))	2GOZ A	32	35	GGAC)))					

PDB code 2QUS; three-way junction (hammerhead)

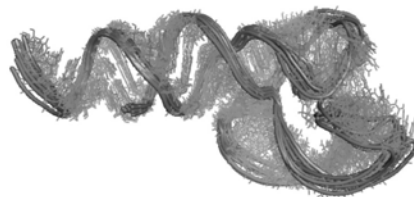
GGGAGCCUGUCACCGAUGUCUUCCGGUCUGAUGAGUCCGUGAGGACAAAACAGGGCUCCCGAAUU
 ((((((((((.((((.....)))))))(.....).(((.....)))).....)))))).....

Input data

Secondary structure derived from the RNA FRABASE
 A square bracket to note U24-A46 interaction was purposefully removed.

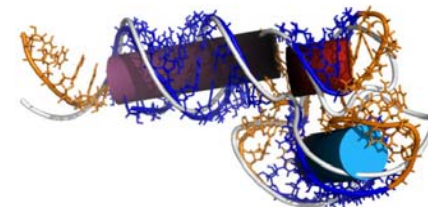


Secondary structure visualization



10 superimposed 3D models

Model No.	Energy [kcal/mol]	r.m.s.d. [Å]
1	-1670	6.4
2	-1620	6.0
3	-1646	6.6
4	-1611	5.9
5	-1664	6.0
6	-1615	7.2
7	-1647	5.9
8	-1643	7.3
9	-1631	7.0
10	-1642	6.5



Lowest r.m.s.d. 3D model (No. 4)

Details of the model No. 4 prediction ^{a)}

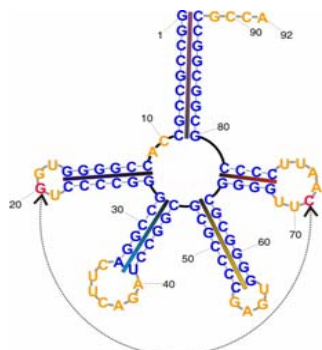
No.	Size [nt]	Target secondary structure element				Source tertiary structure element				Selection criteria					
		localization		secondary structure		localization		secondary structure		secondary structure topology b)	sequence similarity [%] c)	pyrimidines / purines compatibility [%] d)	source structure resolution [Å]	energy [kcal/mol]	
		residues		sequence	topology	PDB ID	residues		sequence						topology
		first	last				first	last							
Single strands															
0	6	64	69	CGAAUU).....	2QUW D	133	138	CGAAUU).....	identical	100.0	100.0	2.2	-78.8
Loops															
1	13	11	13	UCA	((2GOZ B	48	50	UCC	((identical	76.9	84.6	2.2	-267.9
		31	32	UC)	2GOZ A	14	15	GC)					
		37	39	GAG).		20	22	GAG).					
		50	54	CAAAA)...)		35	39	CGAAA)...)					
2	9	18	26	AUGUGCUUU	(.....)	3JYX 5	1691	1699	AUGAGAACU	(.....)	identical	55.6	66.7	8.9	-82.2
3	6	32	37	CUGAUG	(....)	2QUW D	101	106	CUGAUG	(....)	identical	100.0	100.0	2.2	-125.4
4	6	42	47	CGUGAG	(....)	2VQF A	1059	1064	CGUGAG	(....)	identical	100.0	100.0	2.9	-51.7
Stems															
1	22	1	11	GGGAGCCUGU	((((((((2HGU A	15	25	GGGCCACGGU	((((((((identical	54.5	63.6	4.5	-464.9
		54	64	ACAGGGCUCCC)))))))))		541	551	ACCGUGGGCUU)))))))))					
2	12	13	18	ACCGGA	(((3ADB D	120	125	GCCGGA	(((identical	83.3	100.0	2.8	-230.7
		26	31	UCCGGU))))		133	138	UCCGGC))))					
3	2	32	32	C	(single base pair - not used				
		37	37	G)										
4	8	39	42	GUCC	(((3JYX 5	458	461	GUCC	(((identical	100.0	100.0	8.9	-135.5
		47	50	GGAC)))		470	473	GGAC)))					

PDB code 3ADB; five-way-junction (tRNA)

GGCCGCGCCACCGGGGUGGUCCCCGGGCCGGAUCUUCAGAUCCGGCGCGCCCCGAGUGGGGCGCGGGGUCAAUCCCCGCGCGCCGCCA
 ((((((((((...(((...[.]...))))))(((.....))))))(((.....))))))(((.....))))))(((.....)))))).....

Input data

Secondary structure derived from the RNA FRABASE
 Note the square bracket for **G20-C71** loop-loop interaction

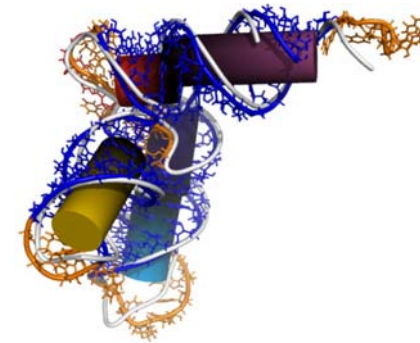


Secondary structure visualization



10 superimposed 3D models

Model No.	Energy [kcal/mol]	r.m.s.d. [Å]
1	-2457	3.9
2	-2446	5.7
3	-2349	6.4
4	-2403	3.6
5	-2365	3.6
6	-2379	5.0
7	-2434	4.4
8	-2408	5.9
9	-2457	3.6
10	-2414	4.9



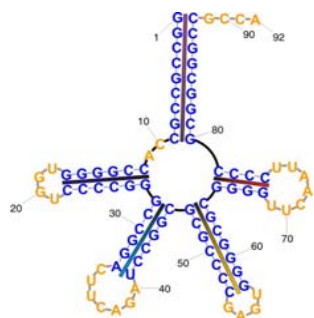
Lowest r.m.s.d. 3D model (No. 4)

Details of the model No. 4 prediction ^{a)}

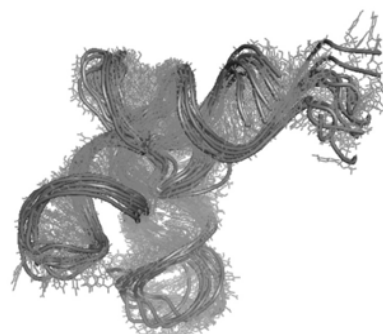
No.	Size [nt]	Target secondary structure element				Source tertiary structure element				Selection criteria					
		localization		secondary structure		localization		secondary structure		secondary structure topology b)	sequence similarity [%] c)	pyrimidines / purines compatibility [%] d)	source structure resolution [Å]	energy [kcal/mol]	
		residues		sequence	topology	PDB ID	residues		sequence						topology
		first	last				first	last							
Single strands															
0	5	88	92	CGCCA)....	3ADC D	180	184	CGCCA)....	identical	100.0	100.0	2.9	-47.9
Loops															
1	12	9	12	CCAC	..(3ADD C	9	12	CCAC	..(identical	100.0	100.0	2.4	-9.2
		27	28	GG)		27	28	GG)					
		46	47	CG)		46	47	CG)					
		64	65	CG)		64	65	CG)					
		79	80	CG)		79	80	CG)					
2	6	17	22	GUGGUC	(.[.]	3ADD C	17	22	GUGGUC	(.[.]	identical	100.0	100.0	2.4	-111.3
3	9	33	41	ACUUCAGAU	(.....)	3ADC D	125	133	ACUUCAGAU	(.....)	identical	100.0	100.0	2.9	-67.1
4	6	53	58	CGAGUG	(....)	3ADD D	145	150	CGAGUG	(....)	identical	100.0	100.0	2.4	-98.3
5	9	68	76	GUUCAAUUC	(.][....)	1ASZ R	52	60	GUUCAAUUC	(.][....)	identical	100.0	100.0	3.0	-165.8
Stems															
1	18	1	9	GGCCGCCG	(((((((3ADC C	1	9	GGCCGCCG	(((((((identical	100.0	100.0	2.9	-349.3
		80	88	GCGGCGCC)))))))))		80	88	GCGGCGCC)))))))))					
2	12	12	17	CCGGGG	((((3ADC D	104	109	CCGGGG	((((identical	100.0	100.0	2.9	-240.5
		22	27	CCCCGG))))		114	119	CCCCGG))))					
3	12	28	33	GCCGGA	((((3ADC C	28	33	GCCGGA	((((identical	100.0	100.0	2.9	-220.5
		41	46	UCCGGC))))		41	46	UCCGGC))))					
4	14	47	53	GCGCCCC	(((((((3ADC D	139	145	GCGCCCC	(((((((identical	100.0	100.0	2.9	-279.7
		58	64	GGGGCGC)))))))))		150	156	GGGGCGC)))))))))					
5	8	65	68	GGGG	(((3FIN A	2598	2601	GGGG	(((identical	100.0	100.0	6.4	-40.7
		76	79	CCCC)))		2730	2733	CCCC)))					

PDB code 3ADB; five-way-junction (tRNA)
 GGCCGCGCCACCGGGGUGGUCCCCGGGCCGGAUCUUCAGAUCCGGCGCGCCCCGAGUGGGGCGCGGGGUCAAUCCCCGCGCGCCGCCA
 (((((((((...((((((.....))))))((((((.....))))))((((((.....))))))((((((.....)))))))))....

Input data
 Secondary structure derived from the RNA FRABASE
 The square bracket to note G20-C71 interaction was removed.

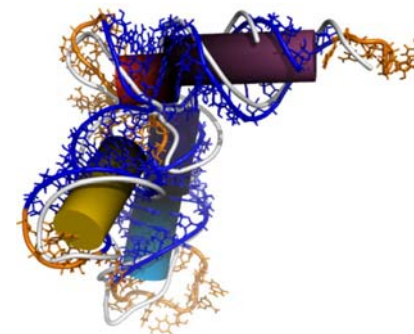


Secondary structure visualization



10 superimposed 3D models

Model No.	Energy [kcal/mol]	r.m.s.d. [Å]
1	-2388	5.1
2	-2333	5.1
3	-2361	6.7
4	-2319	6.3
5	-2393	4.8
6	-2350	4.8
7	-2322	6.3
8	-2372	6.2
9	-2334	5.7
10	-2389	6.7



Lowest r.m.s.d. 3D model (No. 5)

Details of the model No. 5 prediction ^{a)}

No.	Size [nt]	Target secondary structure element				Source tertiary structure element				Selection criteria					
		localization		secondary structure		localization		secondary structure		secondary structure topology b)	sequence similarity [%] c)	pyrimidines / purines compatibility [%] d)	source structure resolution [Å]	energy [kcal/mol]	
		residues		sequence	topology	PDB ID	residues		sequence						topology
		first	last				first	last							
Single strands															
0	5	88	92	CGCCA)....	1FIR A	72	76	CGCCA)....	identical	100.0	100.0	3.3	-46.1
Loops															
1	12	9	12	CCAC	(..(3ADD C	9	12	CCAC	(..(identical	100.0	100.0	2.4	-9.2
		27	28	GG)		27	28	GG)					
		46	47	CG)		46	47	CG)					
		64	65	CG)		64	65	CG)					
		79	80	CG)		79	80	CG)					
2	6	17	22	GUGGUC	(..[.)	3JYX 5	1022	1027	GUCUUC	(.....)	identical	66.7	66.7	8.9	-110.4
3	9	33	41	ACUUCAGAU	(.....)	3ADC D	125	133	ACUUCAGAU	(.....)	identical	100.0	100.0	2.9	-67.1
4	6	53	58	CGAGUG	(.....)	3ADD C	53	58	CGAGUG	(.....)	identical	100.0	100.0	2.4	-13.7
5	9	68	76	GUUCAAUUC	(..[.....)	486D A	52	60	GUUCAAUUC	(.....)	identical	100.0	100.0	7.5	-2.9
Stems															
1	18	1	9	GGCCGCCG	(((((((3ADD D	93	101	GGCCGCCG	(((((((identical	100.0	100.0	2.4	-231.7
		80	88	GCGGCGGC))))))		172	180	GCGGCGGC))))))					
2	12	12	17	CCGGGG	((((3ADD D	104	109	CCGGGG	((((identical	100.0	100.0	2.4	-252.4
		22	27	CCCCGG))))		114	119	CCCCGG))))					
3	12	28	33	GCCGGA	((((3ADC D	120	125	GCCGGA	((((identical	100.0	100.0	2.9	-242.1
		41	46	UCCGGC))))		133	138	UCCGGC))))					
4	14	47	53	GCGCCCC	((((3ADC D	139	145	GCGCCCC	((((identical	100.0	100.0	2.9	-279.7
		58	64	GGGGCG))))		150	156	GGGGCG))))					
5	8	65	68	GGGG	(((3I8F A	2650	2653	GGGG	(((identical	100.0	100.0	3.1	-171.6
		76	79	CCCC)))		2782	2785	CCCC)))					

- a) all the 3D structure elements comprised by the respective crystal PDB structure were excluded from the dictionary
- b) encompassing the structure element size, number and length of RNA strands
- c) similarity between the target and source RNA sequence
- d) shows matching of the purine / pyrimidine residues for the target and source RNA of given sequence

TABLE S7. The quality of 3D models predicted^{a)} for the 5S rRNA *H. Marismortui* (PDB code 1FFK)

<p>Sequence: UUAGCGGGCCACAGCGGUGGGGUUGCCUCCCGUACCCAUCCCGAACACGGAAGAUAGCCCACCAGCGUUCGGGGAGUAC UGGAGUGCGCGAGCCUCUGGGAAACCCGGUUCGCCGCCACC</p>																																																																																																																																						
<p>Input reference secondary structure (RNA FRABASE database): ...(((((((.....((((((((.....(((((((... (... ...)))))...)))))...)))))...))...(((((((... ..(((((((.....)))))...)))))...)))))...)))))))...)</p>			<p>Input determined in this work secondary structure RNAstructure & SHAPE ; MCC^{b)} = 0.99): ...(((((((.....((((((((.....(((((((... (... ...)))))...)))))...)))))...))...(((((((... ..(((((((.....)))))...)))))...)))))...)))))))...)</p>																																																																																																																																			
<p>Prediction output – 10 models.</p> <p>Structure models energy^{c)} and selected parameters defining models quality^{d),e)}</p> <table border="1"> <thead> <tr> <th>Model</th> <th>energy [kcal/mol]</th> <th>r.m.s.d. [Å]</th> <th>INF^{cbp}</th> <th>INF^{all}</th> </tr> </thead> <tbody> <tr><td>1</td><td>-2952</td><td>3.3</td><td>1.00</td><td>0.83</td></tr> <tr><td>2</td><td>n.a.</td><td>3.6</td><td>1.00</td><td>0.83</td></tr> <tr><td>3</td><td>-2920</td><td>5.6</td><td>1.00</td><td>0.81</td></tr> <tr><td>4</td><td>-2902</td><td>4.0</td><td>1.00</td><td>0.82</td></tr> <tr><td>5</td><td>-2960</td><td>3.8</td><td>1.00</td><td>0.83</td></tr> <tr><td>6</td><td>-2903</td><td>3.9</td><td>1.00</td><td>0.81</td></tr> <tr><td>7</td><td>-2871</td><td>4.5</td><td>1.00</td><td>0.79</td></tr> <tr><td>8</td><td>-2881</td><td>3.8</td><td>1.00</td><td>0.82</td></tr> <tr><td>9</td><td>-2865</td><td>3.6</td><td>1.00</td><td>0.81</td></tr> <tr><td>10</td><td>-2925</td><td>3.5</td><td>1.00</td><td>0.83</td></tr> <tr><td colspan="2">mean</td><td>4.0</td><td>1.00</td><td>0.82</td></tr> <tr><td colspan="2">st. dev.</td><td>0.6</td><td>0.00</td><td>0.02</td></tr> </tbody> </table>			Model	energy [kcal/mol]	r.m.s.d. [Å]	INF ^{cbp}	INF ^{all}	1	-2952	3.3	1.00	0.83	2	n.a.	3.6	1.00	0.83	3	-2920	5.6	1.00	0.81	4	-2902	4.0	1.00	0.82	5	-2960	3.8	1.00	0.83	6	-2903	3.9	1.00	0.81	7	-2871	4.5	1.00	0.79	8	-2881	3.8	1.00	0.82	9	-2865	3.6	1.00	0.81	10	-2925	3.5	1.00	0.83	mean		4.0	1.00	0.82	st. dev.		0.6	0.00	0.02	<p>Prediction output – 10 models.</p> <p>Structure models energy^{c)} and selected parameters defining models quality^{d),e)}</p> <table border="1"> <thead> <tr> <th>Model</th> <th>energy [kcal/mol]</th> <th>r.m.s.d. [Å]</th> <th>INF^{cbp}</th> <th>INF^{all}</th> </tr> </thead> <tbody> <tr><td>1</td><td>-2846</td><td>11.4</td><td>0.94</td><td>0.81</td></tr> <tr><td>2</td><td>-2905</td><td>10.9</td><td>1.00</td><td>0.79</td></tr> <tr><td>3</td><td>-2790</td><td>15.1</td><td>0.94</td><td>0.77</td></tr> <tr><td>4</td><td>-2872</td><td>13.2</td><td>0.97</td><td>0.78</td></tr> <tr><td>5</td><td>-2749</td><td>9.4</td><td>0.97</td><td>0.74</td></tr> <tr><td>6</td><td>-2888</td><td>13.1</td><td>1.00</td><td>0.77</td></tr> <tr><td>7</td><td>-2854</td><td>13.7</td><td>0.94</td><td>0.80</td></tr> <tr><td>8</td><td>-2873</td><td>9.5</td><td>0.97</td><td>0.76</td></tr> <tr><td>9</td><td>-2837</td><td>14.1</td><td>0.95</td><td>0.75</td></tr> <tr><td>10</td><td>-2853</td><td>10.6</td><td>0.94</td><td>0.77</td></tr> <tr><td colspan="2">mean</td><td>12.1</td><td>0.96</td><td>0.77</td></tr> <tr><td colspan="2">st. dev.</td><td>1.9</td><td>0.03</td><td>0.03</td></tr> </tbody> </table>		Model	energy [kcal/mol]	r.m.s.d. [Å]	INF ^{cbp}	INF ^{all}	1	-2846	11.4	0.94	0.81	2	-2905	10.9	1.00	0.79	3	-2790	15.1	0.94	0.77	4	-2872	13.2	0.97	0.78	5	-2749	9.4	0.97	0.74	6	-2888	13.1	1.00	0.77	7	-2854	13.7	0.94	0.80	8	-2873	9.5	0.97	0.76	9	-2837	14.1	0.95	0.75	10	-2853	10.6	0.94	0.77	mean		12.1	0.96	0.77	st. dev.		1.9	0.03	0.03
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<p>Time elapsed to generate 10 models: 3 min. 49 sec.</p>			<p>Time elapsed to generate 10 models: 4 min. 15 sec.</p>																																																																																																																																			

- ^{a)} upon validation all the 3D structure elements comprised by the respective crystal PDB structure were excluded from the dictionary
- ^{b)} Matthews correlation coefficient (41) corresponds to the RNA FRABASE secondary structure parsed from the tertiary PDB structure
- ^{c)} potential energy of the final 3D structures were calculated with XPLOR-NIH ver. 2.2 program (26) using parameters from the "dna-rna allatom.param" file
- ^{d)} r.m.s.d. values for all heavy atoms were calculated with XPLOR ver. 2.2 program (26)
- ^{e)} INF^{cbp} describes the interaction network fidelity (33) values over canonical base pairing only; the INF^{all} describes all the base pairing interactions and base stacking. Base pair interactions and base stacking network from tertiary PDB structure were obtained using the RNAView (34) and MC-Annotate (35) programs, respectively.

Table S8. Accuracy of RNA 3D models predicted by RNAComposer, MC-Fold/MC-Sym (21) and iFoldRNA servers (15).

PDB code and chain	Strand length [nt]	RNAComposer			MC-Sym module			iFoldRNA		
		global r.m.s.d. [Å]	INF ^{all}	INF ^{cbp}	global r.m.s.d. [Å]	INF ^{all}	INF ^{cbp}	global r.m.s.d. [Å]	INF ^{all}	INF ^{cbp}
2HW8 B	36	1.7	0.89	1.00	10.8	0.68	1.00	9.5	0.48	0.59
1I6U C	37	2.1	0.90	1.00	2.6	0.83	1.00	4.1	0.62	0.61
1ZHO B	38	1.1	0.83	1.00	10.6	0.76	1.00	11.4	0.58	0.62
2VPL B	48	4.9	0.79	1.00	10.9	0.74	1.00	11.0	0.67	0.78
2PXB B	49	2.5	0.91	1.00	11.1	0.70	1.00	16.2	0.31	0.18
1DK1 B	57	2.4	0.52	0.98	13.2	0.51	1.00	12.5	0.34	0.80
1KXK A	70	9.3	0.74	0.98	10.1	0.69	1.00	10.0	0.58	0.68
3AM1 B	81	5.7	0.78	1.00	12.3	0.76	0.99	21.5	0.54	0.86
Average		3.7	0.80	1.00	10.2	0.71	1.00	12.0	0.52	0.64

Table S9. MolProbity RNA structure stereochemical quality assessment for the 3D models predicted by RNAComposer, MC-Fold/MC-Sym (21) and iFoldRNA (15) servers

PDB code and chain	RNAComposer			MC-Sym module			iFoldRNA		
	clash-score, all atoms	outlier bonds [%]	outlier angles [%]	clash-score, all atoms	outlier bonds [%]	outlier angles [%]	clash-score, all atoms	outlier bonds [%]	outlier angles [%]
2HW8 B	12.90	0.00	0.00	92.78	66.67	91.67	105.74	13.89	77.78
1I6U C	14.31	0.00	0.00	72.33	43.24	97.30	104.86	21.62	72.97
1ZHO B	12.23	0.00	0.00	110.84	71.05	92.11	103.63	21.05	71.05
2VPL B	12.24	0.00	0.00	172.57	79.17	100.00	99.60	22.92	66.67
2PXB B	11.36	0.00	0.00	117.91	71.43	93.88	106.52	22.45	89.80
1DK1 B	19.57	0.00	0.00	125.48	66.67	85.96	109.30	26.32	71.93
1KXK A	19.07	0.00	0.00	95.74	71.43	95.71	110.59	22.86	72.86
3AM1 B	16.08	0.00	0.00	123.61	65.43	90.12	106.55	25.93	71.60
Average	14.72	0.00	0.00	113.91	66.89	93.34	105.85	22.13	74.33

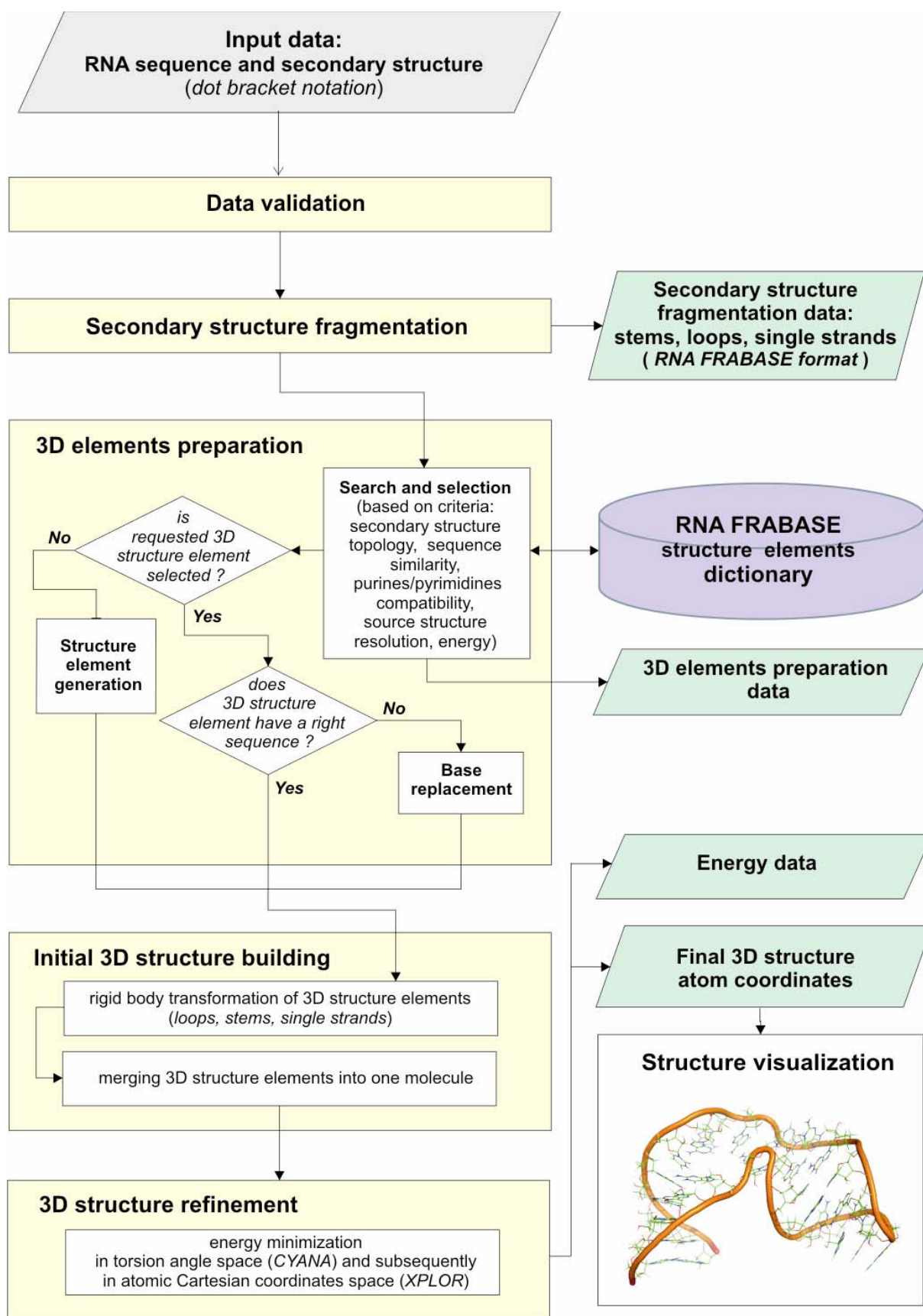


FIGURE S1. Detailed flowchart of the machine translation method to predict RNA 3D structures from secondary structure. User-accessible output files are shown as the rhombohedras (in green)

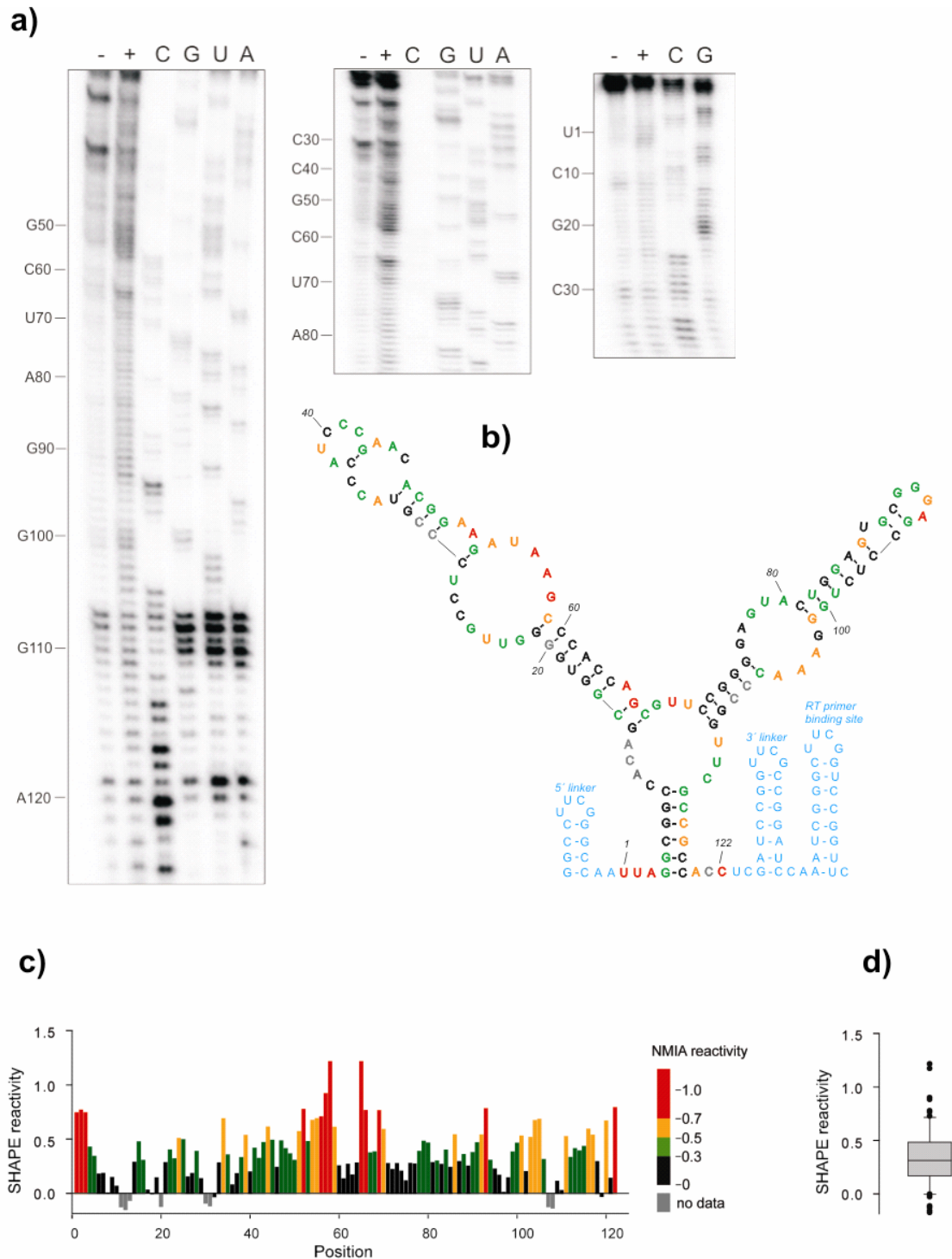


FIGURE S3. Determination of the 5S rRNA *H. Marismortui* secondary structure. **(a)** Typical gel electrophoresis patterns for SHAPE analysis of the 5S rRNA. Lanes (-) represent control sample with untreated RNA; lanes (+) NMIA modification, A, C, G and U are sequencing lanes. **(b)** Secondary structure of the 122-mer 5S rRNA containing 3' structure cassette and 5' flanking sequence to facilitate the analysis of entire RNA by primer extension (36). Nucleotide residues accessibilities to NMIA are given in colours and according to scale. **(c)** Processed SHAPE reactivities as a function of nucleotide position. Red and orange bars reflect reactive positions in the RNA. **(d)** Box plot analysis of distinct reactivity distributions for the 5S rRNA. Box outline middle 50% of dataset; the median is shown with heavy line. Circles indicate extreme values: 1.5 times the interquartile range (boxed). Horizontal lines above and below the box are the largest or smallest non-outlier values.

