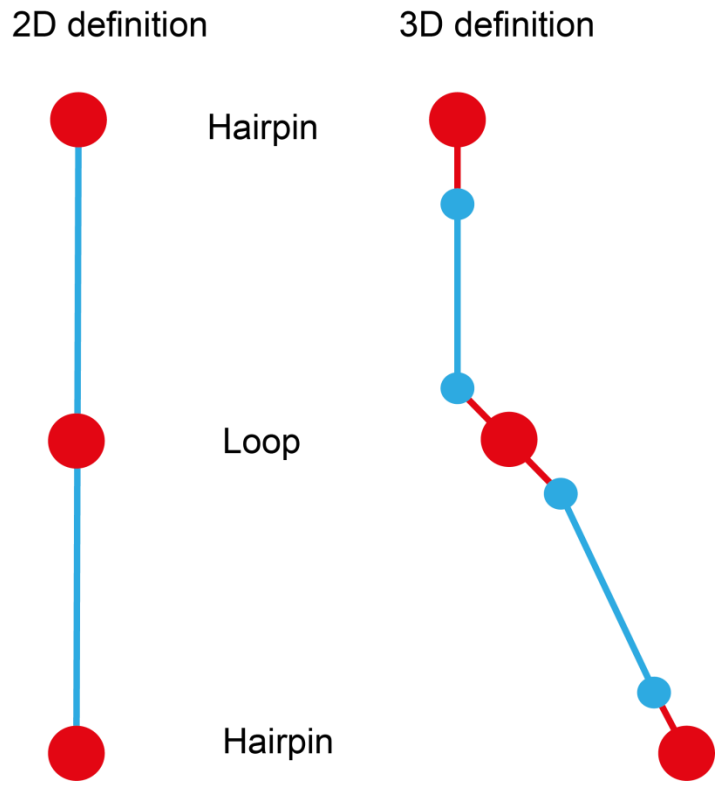
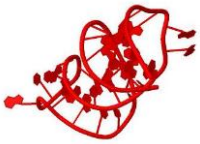
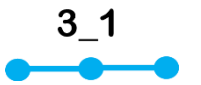
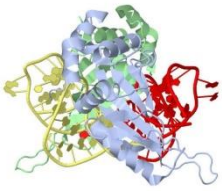
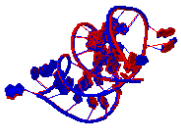
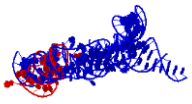
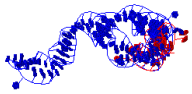
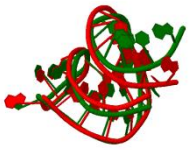
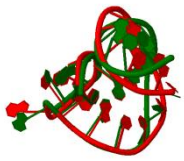
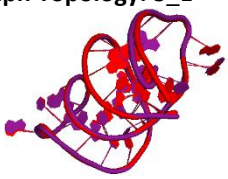
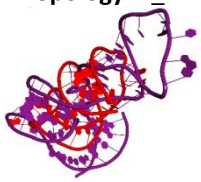
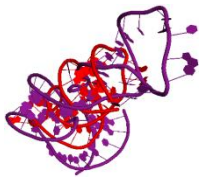


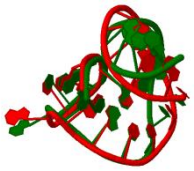
Figure S1. Comparison of 2D and 3D graph representations. In 3D, each helix is represented by one edge and two vertices.

Table S1. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1MJI,C. The five top hits of ARTS sorted by best scores, the five top hits of R3D-BLAST sorted by E-values, and a few top hits of RAG-3D sorted by graph RMSD values for each subgraph ID are listed. The common motifs are highlighted in yellow. The query structure is shown in red in all drawings. The matching structure found by ARTS is shown in blue, the matching segment found by R3D-BLAST is shown in green, and the matching motif found by RAG-3D is shown in purple. The graph topology of each structure is provided. If a structure has more than 10 vertices, its graph topology is given as N/A.

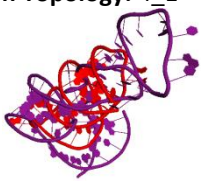
	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1MJI, C  **Molecule:** 5S rRNA fragment of ribosomal protein L5/5S rRNA complex **Graph Topology :** 3_1   1MJI	**1)** 1mji:D 5S rRNA fragment **Score**= 53 **RMSD**= 0.59 **Graph Topology:** 3_1  **2)** 2ho7:AB ribozyme RNA **Score**= 38 **RMSD**= 1.59 **Graph Topology:** 6_2  **3)** 2hgu:A 23S rRNA **Score**= 37 **RMSD**= 1.82 **Graph Topology:** N/A **4)** 1yjw:9 5S rRNA **Score**= 35 **RMSD**= 1.07 **Graph Topology:** 7_3  **5)** 2byt:E	**1)** 4HUB, 9 5S rRNA **E-value**= 6.00E-08 **RMSD**= 2.615 **Graph Topology:** 7_3  **2)** 3J5W, B 5S rRNA **E-value**= 1.00E-07 **RMSD**= 2.562 **Graph Topology:** 4_2  **3)** 3J5U, B 5S rRNA **E-value**= 1.00E-07 **RMSD**= 2.569 **Graph Topology:** 4_2  **4)** 1MJI, D 5S rRNA fragment **E-value**= 2.00E-07 **RMSD**= 2.748 **Graph Topology:** 3_1  **5)** 2I2T, A 5S rRNA	**Subgraph ID 3_1:** **1)** 1MJI, D 5S rRNA fragment **RMSD**= 0.486 **Graph Topology:** 3_1  **2)** 1SJF, B HDV Ribozyme **RMSD**= 1.875 **Graph Topology:** 4_1  **3)** 2OIH, B HDV Ribozyme **RMSD**= 1.876 **Graph Topology:** 4_1  **4)** 1VC7, B HDV Ribozyme **RMSD**= 1.892 **Graph Topology:** 4_1  **5)** 1VBY, B HDV Ribozyme

tRNA
Score= 35
RMSD= 1.58
Graph Topology: 5_3

E-value= 3.00E-07
RMSD= 2.584
Graph Topology: 7_3

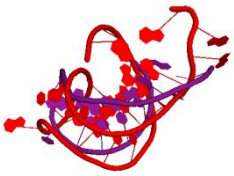


RMSD= 1.916
Graph Topology: 4_1

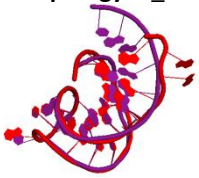


Subgraph ID 2_1 (A):
1) 1MJI, D
5S rRNA fragment
RMSD= 0.277
Graph Topology: 3_1

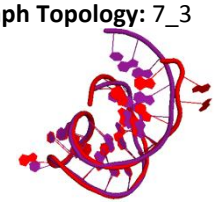
2) 1I6U, D
16S rRNA fragment
RMSD= 1.040
Graph Topology: 3_1



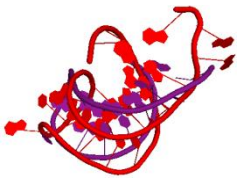
3) 3TVE, B
5S rRNA
RMSD= 1.153
Graph Topology: 7_3



4) 3UZ2, B
5S rRNA
RMSD= 1.163
Graph Topology: 7_3



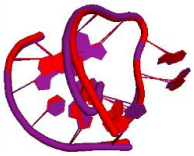
5) 1I6U, C
16S rRNA fragment
RMSD= 1.171
Graph Topology: 3_1



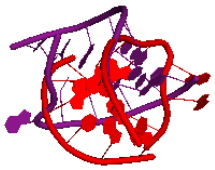
Subgraph ID 2_1 (B):

1) 1N53, AB
T-box RNA
RMSD= 0.477
Graph Topology: 3_1

2) 1MJI, D
5S rRNA fragment
RMSD= 0.501
Graph Topology: 3_1



3) 3CGR, AB
snRNA-branchpoint duplex
RMSD= 0.833
Graph Topology: 3_1

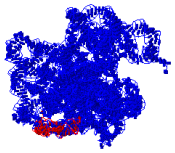
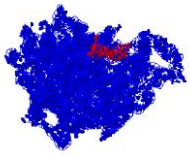
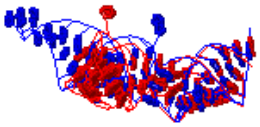
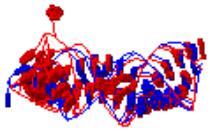
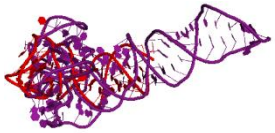


4) 4M6D, D
Aptamer
RMSD= 1.145
Graph Topology: 3_1

5) 3CGQ, AB
snRNA-branchpoint duplex
RMSD= 1.438
Graph Topology: 3_1

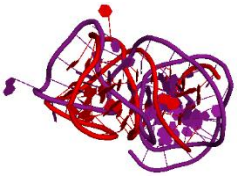
All three tools find the other 5S rRNA fragment, 1MJI,D, which is the other RNA molecule in the asymmetric unit of the structure as a matching structure. ARTS and RAG-3D return it ranked first and R3D-Blast ranks it fourth. R3D-Blast returns five similar 5S rRNAs fragments from larger structures as its top five hits. Interestingly, RAG-3D finds 4 similar HDV ribozymes with 3_1 subgraph IDs as similar structures. RAG-3D also finds many similar substructures of 2_1 subgraph IDs from larger structures such as 5S ribosomal RNAs (3TVE, 3UZ2), a T-box RNA (1N53), and small nuclear (sn)RNAs (3CGQ, 3CGR). There are other common structures found by the three programs but they are in different ranking positions.

Table S2. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1XJR,A. See legend for Table S1.

	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1XJR,A  **Molecule:** the stem-loop II motif (s2m) RNA element of the SARS virus genome **Graph Topology :** 5_1 **5_1**   1XJR	**1)** 2i2u:A 16S rRNA **Score**= 56 **RMSD**= 1.31 **Graph Topology:** N/A  **2)** 2hgu:A 23S rRNA **Score**= 48 **RMSD**= 1.80 **Graph Topology:** N/A  **3)** 1hq1:B SRP RNA **Score**= 47 **RMSD**= 1.33 **Graph Topology:** 4_1  **4)** 1i6u:D 16S rRNA fragment **Score**= 47 **RMSD**= 1.59 **Graph Topology:** 3_1  **5)** 1s03:B 44-mer RNA **Score**= 44 **RMSD**= 1.61 **Graph Topology:** 3_1	none	**Subgraph ID 5_1:** **1)** 1HR2, A Ribozyme **RMSD**= 8.193 **Graph Topology:** 10_2  **2)** 1L8V, B Ribozyme **RMSD**= 8.325 **Graph Topology:** 10_2  **3)** 3J46, 4 23S rRNA **RMSD**= 8.342 **Graph Topology:** 5_1  **4)** 1L8V, A Ribozyme **RMSD**= 8.346 **Graph Topology:** 10_2  **5)** 4K27, U Myotonic Dystrophy Type 2 RNA **RMSD**= 8.417 **Graph Topology:** 6_1

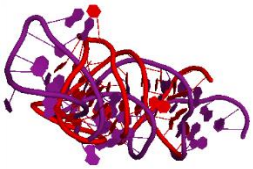
Subgraph ID 4_1 (A):

1) 3E1D, A
5S rRNA
RMSD= 4.446
Graph Topology: 7_2



2) 3J46, 4
23S rRNA
RMSD= 4.570
Graph Topology: 5_1

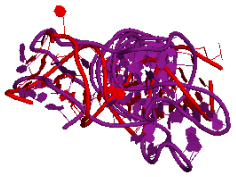
3) 3J2C, O
16S rRNA
RMSD= 4.645
Graph Topology: 8_1



Subgraph ID 4_1 (B):

1) 4K27, U
Myotonic Dystrophy Type 2 RNA
RMSD= 5.276
Graph Topology: 6_1

2) 3J46, 4
23S rRNA
RMSD= 5.424
Graph Topology: 5_1

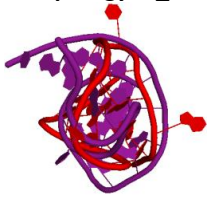


3) 3IZZ, A
Helix
RMSD= 5.721
Graph Topology: 4_1

Subgraph ID 3_1 (A):
1) 1NTA, AB
Streptomycin RNA-aptamer
RMSD= 3.061
Graph Topology: 4_1

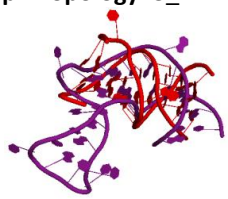
2) 3P59, ABCDEFGH
RNA Nanosquare
RMSD= 3.405
Graph Topology: 3_1

3) 4KQY, A
S box/SAM-I riboswitch
RMSD= 3.617
Graph Topology: 8_2

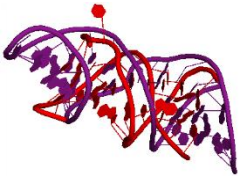


Subgraph ID 3_1 (B):
1) 1KP7, A
HCV IRES fragment
RMSD= 2.564
Graph Topology: 3_1

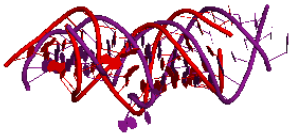
2) 2OZB, C
snRNA
RMSD= 2.570
Graph Topology: 3_1



3) 2LPT, A
34-mer RNA
RMSD= 2.573
Graph Topology: 3_1



Subgraph ID 3_1 (C):
1) 2PXL, B
4.5 S RNA
RMSD= 2.085
Graph Topology: 4_1



2) 4JRC, B
T-box RNA
RMSD= 2.705
Graph Topology: 4_1

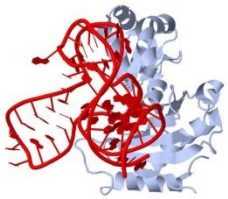
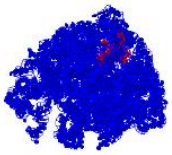
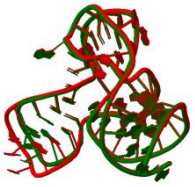
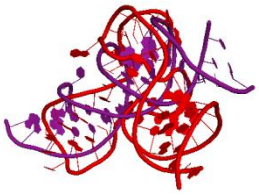
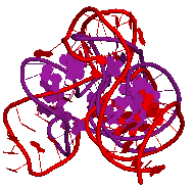
3) 4JRC, A
T-box RNA
RMSD= 2.921
Graph Topology: 4_1

Subgraph ID 2_1 (A):
1) 2B9M, V
tRNA
RMSD= 0.675
Graph Topology: 3_1

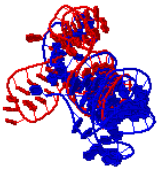
Subgraph ID 2_1 (B):
1) 1ZE2, D
RNA substrate
RMSD= 0.497
Graph Topology: 2_1

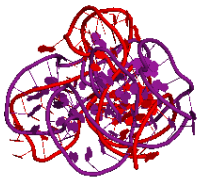
R3D-Blast fails to produce a matching structure. RAG-3D finds similar 5_1 motifs but their graph RMSD values are greater than 8. Thus, we may conclude that the s2m RNA has a very unique structure. On the other hand, RAG-3D can find many similar 2_1 motifs from large structures (e.g., 2B9M, 1ZE2) that do not overlap with 4_1 or 3_1 substructures. First two hits of ARTS are not included in RAG database since they have more than 10 vertices.

Table S3. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1MZP,B. See legend for Table S1.

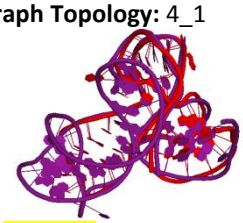
	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1MZP, B  **Molecule:** 55-nucleotide fragment of 23S rRNA in complex with ribosomal protein L1 **Graph Topology :** 4_1   1MZP	**1)** 2hgu:A 23S rRNA **Score**= 44 **RMSD**= 1.65 **Graph Topology:** N/A  **2)** 2drb:B tRNA **Score**= 42 **RMSD**= 1.57 **Graph Topology:** 2_1  **3)** 1d4r:AB SRP RNA **Score**= 41 **RMSD**= 1.20 **Graph Topology:** 5_1  **4)** 486d:C tRNA **Score**= 41 **RMSD**= 1.72 **Graph Topology:** 5_3  **5)** 1kxk:A group II intron **Score**= 40 **RMSD**= 1.45	**1)** 2NOQ, E 25S rRNA **E-value**= 9.00E-29 **RMSD**= 1.233 **Graph Topology:** 4_1  **2)** 2Y0Z, A 23S rRNA **E-value**= 2.00E-10 **RMSD**= 1.565 **Graph Topology:** N/A  **3)** 1PNU, 0 23S rRNA **E-value**= 1.00E-08 **RMSD**= 0.001 **Graph Topology:** N/A  **4)** 1PNY, 0 23S rRNA **E-value**= 1.00E-08 **RMSD**= 0.001 **Graph Topology:** N/A  **5)** 2Y19, A 23S rRNA **E-value**= 1.00E-08 **RMSD**= 1.708 **Graph Topology:** N/A	**Subgraph ID 4_1:** **1)** 2NOQ, E 25S rRNA **RMSD**= 0.002 **Graph Topology:** 4_1  **2)** 4K27, U Myotonic Dystrophy Type 2 RNA **RMSD**= 3.835 **Graph Topology:** 6_1  **3)** 3IZZ, E Helix **RMSD**= 4.106 **Graph Topology:** 7_1  **4)** 2NOQ, B 18S rRNA **RMSD**= 4.701 **Graph Topology:** 4_1  **5)** 2WWA, D 25S rRNA **RMSD**= 4.804 **Graph Topology:** 4_1

Graph Topology: 5_1

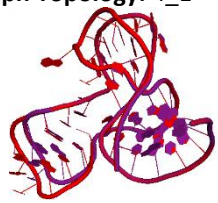




Subgraph ID 3_1 (A):
1) 4BYQ, N
L1 rRNA
RMSD= 1.128
Graph Topology: 4_1



2) 2NOQ, E
25S rRNA
RMSD= 1.620
Graph Topology: 4_1



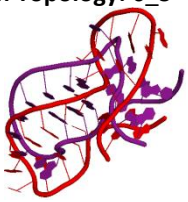
3) 3J44, 3
5S rRNA
RMSD= 3.597
Graph Topology: 7_3

Subgraph ID 3_1 (B):
1) 2NOQ, E
25S rRNA
RMSD= 0.002
Graph Topology: 4_1

2) 3UMY, B
23S rRNA fragment
RMSD= 0.782
Graph Topology: 5_1

3) 3U56, B
23S rRNA fragment
RMSD= 1.054
Graph Topology: 5_1

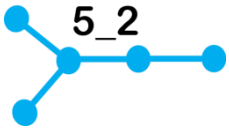
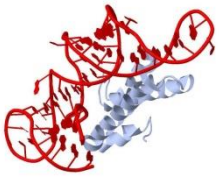
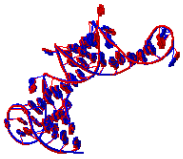
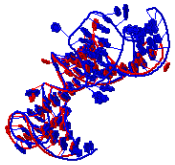
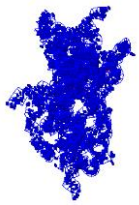
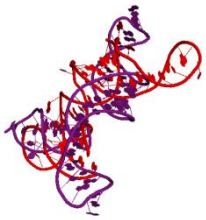
Subgraph ID 2_1 (A):
1) 3IQP, A
SAM-I riboswitch
RMSD= 0.678
Graph Topology: 6_5



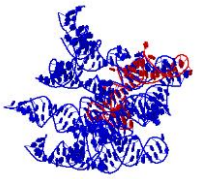
Subgraph ID 2_1 (B):
1) 2NOQ, E
25S rRNA
RMSD= 0.002
Graph Topology: 4_1

Both R3D-Blast and RAG-3D find 25S ribosomal RNA 2NOQ,E of the ribosome-bound cricket paralysis virus IRES (internal ribosome entry site) RNA as the best matching result but the other results differ. As well as this similar structure of 4_1 topology ID, RAG-3D finds smaller matching substructures of 3_1 and 2_1 topology IDs from different structures such as a fragment of 23S RNA in complex with different mutants of ribosomal protein tthl1 (3UMY,B and 3U56,B) and a SAM-I riboswitch, 3IQP,A.

Table S4. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1DK1,B. See legend for Table S1.

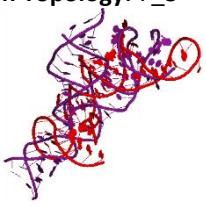
	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1DK1, B  **Molecule:** 16S rRNA fragment of the ribosomal protein S15-rRNA complex **Graph Topology :** 5_2   1DK1	**1)** 1kuq:B 16S rRNA fragment **Score**= 99 **RMSD**= 0.56 **Graph Topology:** 5_2  **2)** 2i2u:A 16S rRNA **Score**= 81 **RMSD**= 1.61 **Graph Topology:** N/A  **3)** 1g1x:DE 16S rRNA **Score**= 78 **RMSD**= 1.25 **Graph Topology:** 6_2  **4)** 1yl4:A1 16S rRNA-mRNA **Score**= 77 **RMSD**= 1.72 **Graph Topology:** N/A 	**1)** 1KUQ, B 16S rRNA fragment **E-value**= 2.00E-19 **RMSD**= 1.568 **Graph Topology:** 5_2  **2)** 1F7Y, B 16S rRNA fragment **E-value**= 2.00E-15 **RMSD**= 0.747 **Graph Topology:** 5_2  **3)** 1F7Y, B 16S rRNA fragment **E-value**= 3.00E-11 **RMSD**= 0.183 **Graph Topology:** 5_2  **4)** 2UUC, A 16S rRNA **E-value**= 0.001 **RMSD**= 1.295 **Graph Topology:** N/A 	**Subgraph ID 5_2:** **1)** 1F7Y, B 16S rRNA fragment **RMSD**= 0.037 **Graph Topology:** 5_2  **2)** 1KUQ, B 16S rRNA fragment **RMSD**= 0.322 **Graph Topology:** 5_2  **3)** 2OIU, P L1 Ribozyme **RMSD**= 5.138 **Graph Topology:** 6_3  **4)** 3IZD, A rRNA **RMSD**= 6.373 **Graph Topology:** 9_4 

5) 2a64:A
Ribonuclease P RNA
Score=47
RMSD= 1.81
Graph Topology: N/A



5) 2VQE, A
16S rRNA
E-value= 0.001
RMSD= 1.332
Graph Topology: N/A

5) 1Y69, 9
5S rRNA
RMSD= 7.811
Graph Topology: 7_3



Subgraph ID 4_2:
1) 1F7Y, B
16S rRNA fragment
RMSD= 0.037
Graph Topology: 5_2

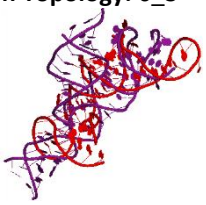
2) 1KUQ, B
16S rRNA fragment
RMSD= 0.299
Graph Topology: 5_2

3) 2OIU, P
L1 Ribozyme
RMSD= 5.138
Graph Topology: 6_3

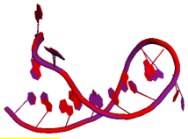
4) 3CUL, C
92-mer RNA
RMSD= 6.519
Graph Topology: 5_2

5) 3CUN, C
92-mer RNA

RMSD= 7.228
Graph Topology: 6_3

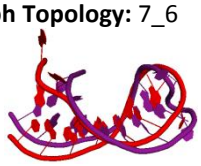


Subgraph ID 2_1:
1) 1F7Y, B
16S rRNA fragment
RMSD= 0.104
Graph Topology: 5_2

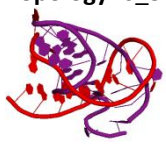


2) 1KUQ, B
16S rRNA fragment
RMSD= 0.322
Graph Topology: 5_2

3) 3J62, C
5.8S rRNA
RMSD= 0.644
Graph Topology: 7_6



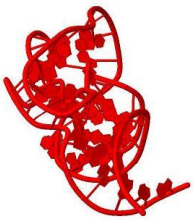
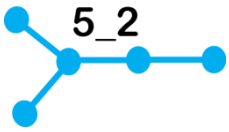
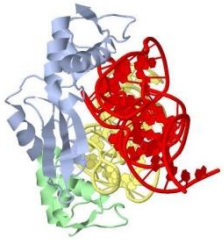
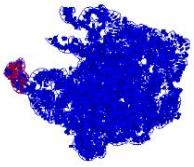
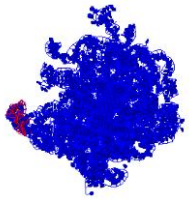
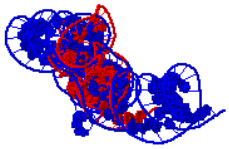
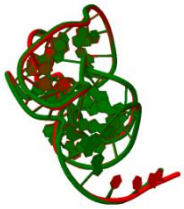
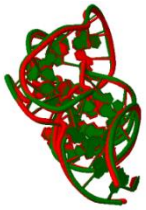
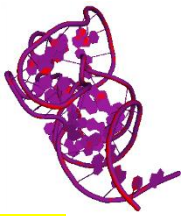
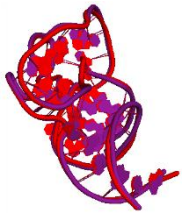
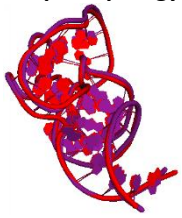
4) 2HOO, A
Thi-box riboswitch
RMSD= 0.704
Graph Topology: 6_3



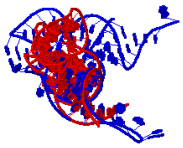
5) 1F9L, A
22-mer RNA
RMSD= 0.729
Graph Topology: 3_1

All three tools return 1KUQ,B which is Thr3Cys mutant ribosomal protein S15 in complex with 16S rRNA as a matching result. Both R3D-Blast and RAG-3D also find the same rRNA structure, 1F7Y,B, from the structure of two UUCG loops embedded in the same complex and present it in different order because of different ordering parameters. Both ARTS and R3D-BLAST find matching 16S rRNA structures from large complex structures which are not included in RAG-3D database since they have more than 10 vertices. 1DK1 has a 3-way junction structure and RAG-3D finds RNAs sharing a similar 3-way junction structure such as 2OIU,P. Interestingly, RAG-3D finds similar 2_1 motifs such as the thi-box riboswitch bound to benfotiamine, 2HOO,A, and 22 nt RNA hairpin, 1F9L, A.

Table S5. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1MMS,C. See legend for Table S1.

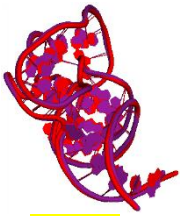
	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1MMS, C  **Molecule:** a fragment of 23S rRNA bound to ribosomal protein L11 **Graph Topology :** 5_2   1MMS	**1)** 1vqm:40 23S rRNA **Score**= 92 **RMSD**= 0.98 **Graph Topology:** N/A  **2)** 2i2v:B 23S rRNA **Score**= 89 **RMSD**= 1.23 **Graph Topology:** N/A  **3)** 2gis:A SAM-I riboswitch **Score**= 40 **RMSD**= 1.63 **Graph Topology:** 7_7  **4)** 1mfq:A SRP RNA **Score**= 38 **RMSD**= 1.93 **Graph Topology:** 9_19  **5)** 1qf6:B tRNA **Score**= 37 **RMSD**= 1.38	**1)** 1OLN, C rRNA fragment **E-value** = 2.00E-39 **RMSD**= 0 **Graph Topology:** 5_2  **2)** 1MMS, D 23S rRNA fragment **E-value** = 3.00E-35 **RMSD**= 0.362 **Graph Topology:** 5_2  **3)** 2QBI, B 23S rRNA **E-value** = 5.00E-30 **RMSD**= 0.753 **Graph Topology:** 7_3  **4)** 1C04, E 23S rRNA fragment **E-value** = 4.00E-29 **RMSD**= 0.66 **Graph Topology:** 5_2  **5)** 1QA6, C 58-mer rRNA **E-value** = 4.00E-29 **RMSD**= 0.66	**Subgraph ID 5_2:** **1)** 1OLN, C rRNA fragment **RMSD**= 0.000 **Graph Topology:** 5_2  **2)** 1MMS, D 23S rRNA fragment **RMSD**= 0.054 **Graph Topology:** 5_2  **3)** 1Y39, C 58-mer rRNA **RMSD**= 0.457 **Graph Topology:** 5_2  **4)** 1HC8, D 58-mer rRNA **RMSD**= 0.511 **Graph Topology:** 5_2  **5)** 1QA6, C 58-mer rRNA **RMSD**= 0.534 **Graph Topology:** 5_2

Graph Topology: 5_3

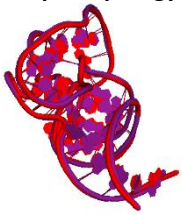


Graph Topology: 5_2

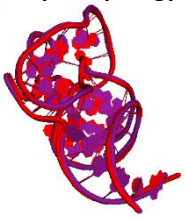
6) 1QA6, D
58-mer rRNA
E-value = 4.00E-29
RMSD= 0.66
Graph Topology: 5_2



6) 1QA6, D
58-mer rRNA
RMSD= 0.534
Graph Topology: 5_2



7) 1C04, E
23S rRNA fragment
RMSD= 0.534
Graph Topology: 5_2



Subgraph ID 4_2:
1) 1OLN, C
rRNA fragment
RMSD= 0.000
Graph Topology: 5_2

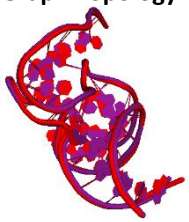
2) 1Y39, C
58-mer rRNA
RMSD= 0.472
Graph Topology: 5_2

3) 1QA6, C
58-mer rRNA
RMSD= 0.552

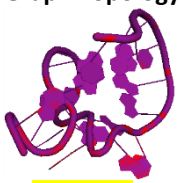
Graph Topology: 5_2

4) 1QA6, D
58-mer rRNA
RMSD= 0.552
Graph Topology: 5_2

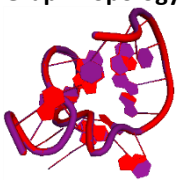
5) 1C04, E
23S rRNA fragment
RMSD= 0.546
Graph Topology: 5_2



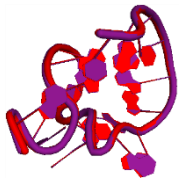
Subgraph ID 2_1:
1) 1OLN, C
rRNA fragment
RMSD= 0.000
Graph Topology: 5_2



2) 1MMS, D
23S rRNA
RMSD= 0.063
Graph Topology: 5_2



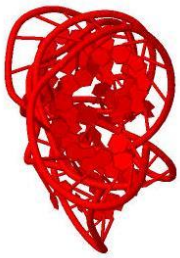
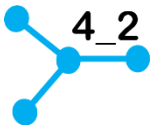
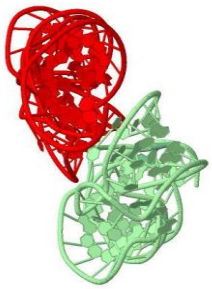
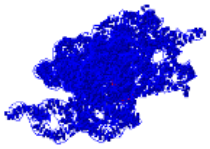
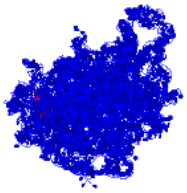
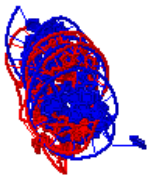
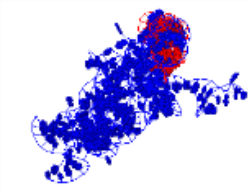
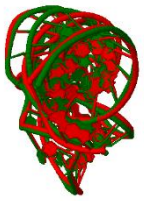
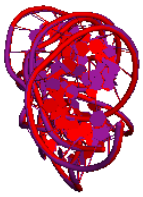
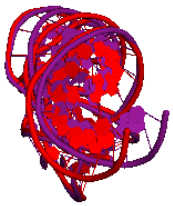
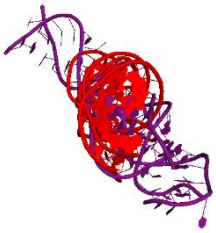
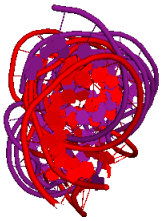
3) 3DEG, G
50S RNA helix
RMSD= 0.183
Graph Topology: 5_2

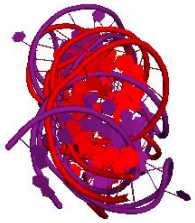


Both R3D-Blast and RAG-3D find 1OLN,C and 1MMS,D of topology ID 5_2 as matching results. 1OLN is the structure of thiostrepton antibiotic binding to the same L11-RNA complex. 1MMS,D is the other RNA molecule in the asymmetric unit of the structure. All other results returned by RAG-3D and R3D-Blast are the same L11 protein binding RNAs. Thus, both programs can successfully return the same substructures. 1C04,E, as well as the symmetric C and D chains of 1QA6 are the same 23S rRNA fragments and thus have the same RMSD values. These structures returned by R3D-Blast in positions 4-6 and by RAG-3D in positions 5-7. The third and fourth hits of RAG-3D which are also 23S rRNA fragments (1Y39, and 1HC8) are also found by R3D-Blast but they are listed in lower positions when the results are ordered by E-values.

ARTS again returns a completely different list. Some of these structures are not included in our dataset since they have more than 10 vertices and some of them are not listed here since they have large RMSD values. The fourth hit of ARTS, 1MFQ,A, and the query RNA share a similar 3-way Family A junction structure whereas the third hit, 2GIS,A, has 4-way junction structure.

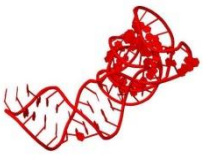
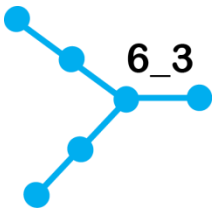
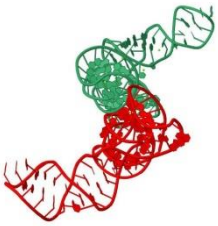
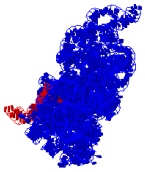
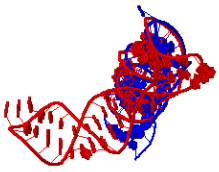
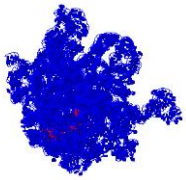
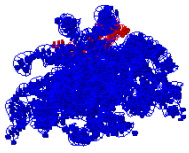
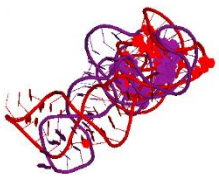
Table S6. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 2QUS,A. See legend for Table S1.

	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 2QUS, A  **Molecule:** Hammerhead ribozyme **Graph Topology :** 4_2   2QUS	**1)** 1yl4:A1 16S rRNA-mRNA **Score**= 63 **RMSD**= 1.83 **Graph Topology:** N/A  **2)** 2i2v:B 23S rRNA **Score**= 60 **RMSD**= 1.75 **Graph Topology:** N/A  **3)** 2f8t:DC 26-mer RNA **Score**= 58 **RMSD**= 1.35 **Graph Topology:** 2_1  **4)** 2a64:A Ribonuclease P RNA **Score**= 54 **RMSD**= 1.59 **Graph Topology:** N/A 	**1)** 2QUW, B Hammerhead ribozyme **E-value**= 7.00E-28 **RMSD**= 0.411 **Graph Topology:** 4_2  **2)** 2QUS, B Hammerhead ribozyme **E-value**= 2.00E-20 **RMSD**= 1.693 **Graph Topology:** 4_2  **3)** 2QUW, D Hammerhead ribozyme **E-value**= 4.00E-09 **RMSD**= 2.311 **Graph Topology:** 4_2  **4)** 3ZD4, A Hammerhead ribozyme **E-value**= 0.0007 **RMSD**= 2.045 **Graph Topology:** 2_1 	**Subgraph ID 4_2:** **1)** 2QUW, AB Hammerhead ribozyme **RMSD**= 0.251 **Graph Topology:** 4_2  **2)** 2QUS, B Hammerhead ribozyme **RMSD**= 1.102 **Graph Topology:** 4_2  **3)** 3J12, A 5S rRNA **RMSD**= 5.059 **Graph Topology:** 8_10  **4)** 3SKI, B 68-mer RNA **RMSD**= 5.059 **Graph Topology:** 4_2 

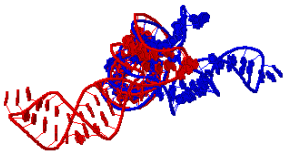
	5) 2nz4:FQ GlmS ribozyme-substrate **Score**= 53 **RMSD**= 1.47 **Graph Topology:** 6_5 	**5)** 3ZP8, A Hammerhead ribozyme **E-value**= 0.002 **RMSD**= 1.736 **Graph Topology:** 2_1 	**5)** 3LA5, A Riboswitch **RMSD**= 6.397 **Graph Topology:** 4_2 

2QUS and 2QUW are the structures of a hammerhead ribozyme pre-cleavage (enzyme-substrate complex) and after cleavage (enzyme-product complex), respectively. R3D-Blast and RAG-3D return same top 2 matching structures; the other chain of the same structure 2QUS,B and the same ribozyme after cleavage, 2QUW. RAG-3D searches only for similar structures with 4_2 motifs since junction is the basic module and it has no smaller subgraphs.

Table S7. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 2OIU,P. See legend for Table S1.

	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 2OIU, P  **Molecule:** L1 Ribozyme RNA Ligase **Graph Topology :** 6_3   2OIU	**1)** 1yl4:A1 16S rRNA-mRNA **Score**= 53 **RMSD**= 1.59 **Graph Topology:** N/A  **2)** 2f8t:DC 26-mer RNA **Score**= 50 **RMSD**= 1.42 **Graph Topology:** 2_1  **3)** 2hgu:A 23S rRNA **Score**= 49 **RMSD**= 1.49 **Graph Topology:** N/A  **4)** 2i2u:A 16S rRNA **Score**= 49 **RMSD**= 1.50 **Graph Topology:** N/A  **5)** 2oiu:Q L1 Ribozyme **Score**= 48	**1)** 2OIU, Q L1 Ribozyme **E-value**= 0.0005 **RMSD**= 12.002 **Graph Topology:** 6_3 	**Subgraph ID 6_3:** **1)** 3HUZ, B 5S rRNA **RMSD**= 7.687 **Graph Topology:** 6_3  **2)** 4GAR, B 5S rRNA **RMSD**= 7.771 **Graph Topology:** 6_3  **3)** 3OFQ, B 5S rRNA **RMSD**= 8.111 **Graph Topology:** 6_3  **4)** 2OIU, Q L1 Ribozyme **RMSD**= 8.441 **Graph Topology:** 6_3  **5)** 3NDB, M SRP RNA **RMSD**= 8.715 **Graph Topology:** 8_10

RMSD= 0.89
Graph Topology: 6_3



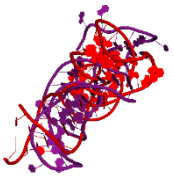
Subgraph ID 5_2 (A):
1) 1KUQ, B
16S rRNA fragment
RMSD= 5.022
Graph Topology: 5_2

2) 1F7Y, B
16S rRNA fragment
RMSD= 5.116
Graph Topology: 5_2

3) 1DK1, B
rRNA fragment
RMSD= 5.138
Graph Topology: 5_2

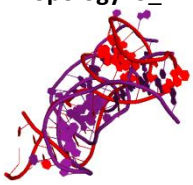
Subgraph ID 5_2 (B):
1) 1KUQ, B
16S rRNA fragment
RMSD= 5.022
Graph Topology: 5_2

2) 1F7Y, B
16S rRNA fragment
RMSD= 5.116
Graph Topology: 5_2

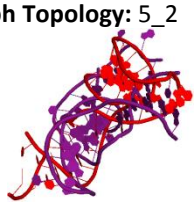


3) 1DK1, B
rRNA fragment
RMSD= 5.138
Graph Topology: 5_2

Subgraph ID 4_2:
1) 1KUQ, B
16S rRNA fragment
RMSD= 5.022
Graph Topology: 5_2



2) 1F7Y, B
16S rRNA fragment
RMSD= 5.116
Graph Topology: 5_2



3) 1DK1, B
rRNA fragment
RMSD= 5.138
Graph Topology: 5_2

Subgraph ID 2_1 (A):
1) 4C8Y, C
R1 REPEAT RNA SUBSTRATE MIMIC
RMSD= 0.002
Graph Topology: 2_1

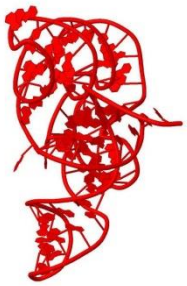
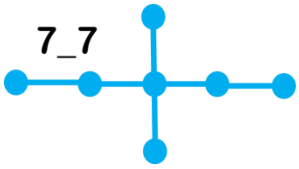
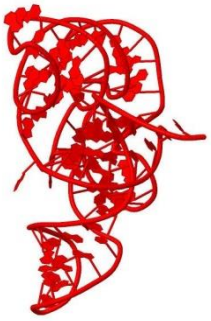
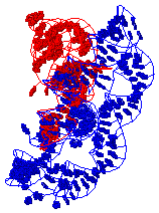
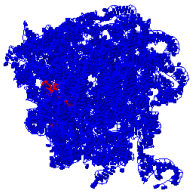
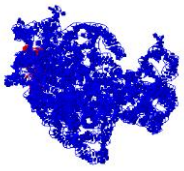
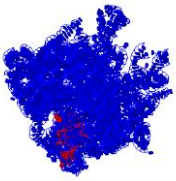
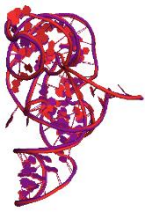
2) 2OEU, A
Hammerhead ribozyme
RMSD= 0.007
Graph Topology: 2_1

Subgraph ID 2_1 (B):
1) 1L9A, B
SRP RNA
RMSD= 0.574
Graph Topology: 8_10

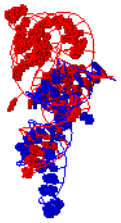
2) 3JYX, 4
5.8S rRNA
RMSD= 0.675
Graph Topology: 3_1

All three tools find 2OIU,Q which is the other chain of the L1 ribozyme structure as a matching result. ARTS finds it in ranking 5, R3D-Blast as first, and RAG-3D in position 4 in 6_3 motifs. R3D-Blast returns only one result and the results of RAG-3D of large topologies 6_3, 5_2, and 4_2 have large RMSD values. Therefore, we may conclude that this structure has a unique structure. However, RAG-3D finds many similar substructures of 2_1 topology IDs such as a CRISPR (4C8Y,C), a hammerhead ribozyme (2OEU,A), RNA structure within the signal recognition particle (SRP) RNA (1L9A,B), and the 5.8 ribosomal RNA (3JYX,4). Three of the results of ARTS are not found by RAG-3D since they are not included in the database.

Table S8. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 2GIS,A. See legend for Table S1.

	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 2GIS, A  **Molecule:** SAM-I riboswitch **Graph Topology :** 7_7   2GIS	**1)** 2nz4:FQ GlmS ribozyme-substrate **Score**= 55 **RMSD**= 1.48 **Graph Topology:** 6_5  **2)** 2i2v:B 23S rRNA **Score**= 52 **RMSD**= 1.67 **Graph Topology:** N/A  **3)** 2i2u:A 16S rRNA **Score**= 52 **RMSD**= 1.95 **Graph Topology:** N/A  **4)** 1vqm:40 23S rRNA **Score**= 48 **RMSD**= 1.97 **Graph Topology:** N/A 	**1)** 3GX5, A SAM-I riboswitch **E-value**= 1.00E-40 **RMSD**= 0.517 **Graph Topology:** 7_7  **2)** 3GX3, A SAM-I riboswitch **E-value**= 3.00E-40 **RMSD**= 0.828 **Graph Topology:** 7_7  **3)** 3IQN, A SAM-I riboswitch **E-value**= 5.00E-40 **RMSD**= 0.746 **Graph Topology:** 7_7  **4)** 3GX6, A SAM-I riboswitch **E-value**= 5.00E-40 **RMSD**= 0.884 **Graph Topology:** 6_5 	**Subgraph ID 7_7:** **1)** 3GX5, A SAM-I riboswitch **RMSD**= 0.266 **Graph Topology:** 7_7  **2)** 3GX3, A SAM-I riboswitch **RMSD**= 0.342 **Graph Topology:** 7_7  **3)** 3GX2, A SAM-I riboswitch **RMSD**= 0.369 **Graph Topology:** 7_7  **4)** 2YDH, A SAM-I riboswitch **RMSD**= 0.421 **Graph Topology:** 7_7 

5) 1hq1:B
SRP RNA
Score= 45
RMSD= 1.40
Graph Topology: 4_1



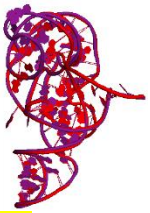
5) 2YGH, A
SAM-I riboswitch
E-value= 9.00E-39
RMSD= 1.405
Graph Topology: 7_7

5) 3IQN, A
SAM-I riboswitch
RMSD= 0.455
Graph Topology: 7_7

Subgraph ID 6_5 (A):
1) 3GX5, A
SAM-I riboswitch
RMSD= 0.261
Graph Topology: 7_7

2) 3GX2, A
SAM-I riboswitch
RMSD= 0.384
Graph Topology: 7_7

3) 2YDH, A
SAM-I riboswitch
RMSD= 0.387
Graph Topology: 7_7



4) 3IQN, A
SAM-I riboswitch
RMSD= 0.388
Graph Topology: 7_7

Subgraph ID 6_5 (B):
1) 3GX5, A
SAM-I riboswitch
RMSD= 0.278
Graph Topology: 7_7

2) 3GX3, A
SAM-I riboswitch
RMSD= 0.332
Graph Topology: 7_7

3) 3GX2, A
SAM-I riboswitch
RMSD= 0.373
Graph Topology: 7_7

4) 2YDH, A
SAM-I riboswitch
RMSD= 0.387
Graph Topology: 7_7

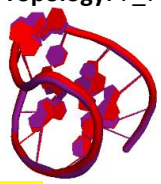
Subgraph ID 5_3:
1) 3GX5, A

SAM-I riboswitch
RMSD= 0.275
Graph Topology: 7_7

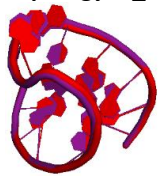
2) 2YDH, A
SAM-I riboswitch
RMSD= 0.387
Graph Topology: 7_7

3) 3GX2, A
SAM-I riboswitch
RMSD= 0.390
Graph Topology: 7_7

Subgraph ID 2_1 (A):
1) 3GX2, A
SAM-I riboswitch
RMSD= 0.169
Graph Topology: 7_7



2) 3GX5, A
SAM-I riboswitch
RMSD= 0.196
Graph Topology: 7_7

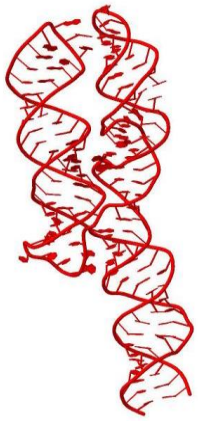
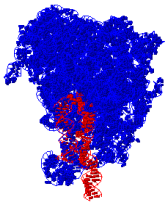
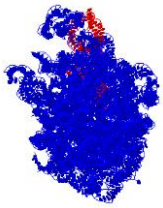


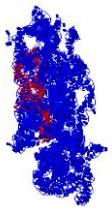
3) 4AOB, A
SAM-I riboswitch

			RMSD= 0.212 **Graph Topology:** 7_7  **Subgraph ID 2_1 (B):** **1)** 3IQN, A SAM-I riboswitch **RMSD**= 0.209 **Graph Topology:** 7_7  **2)** 2YDH, A SAM-I riboswitch **RMSD**= 0.283 **Graph Topology:** 7_7  **3)** 3GX2, A SAM-I riboswitch **RMSD**= 0.306 **Graph Topology:** 7_7 

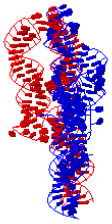
Both R3D-Blast and RAG-3D return similar results whereas ARTS return a different set. The structures of SAM-I riboswitch bound with SAM (3GX5,A), SAM-I riboswitch bound with SAH (3GX3,A), the ligand-free form of the SAM-I riboswitch (3IQN,A), SAM-I riboswitch bound with SAM in manganese chloride (3GX6,A), SAM-I riboswitch bound to sinefungin (3GX2,A), and SAM-I riboswitch in comlex with SAM (2YDH,A) are all found by both R3D-Blast and RAG-3D in different rankings. RAG-3D returns another SAM-I riboswitch, 4AOB, in the matching list of 2_1 topology ID, which is not returned by other tools. On the other hand, ARTS return the structure of the GlmS ribozyme bound to its catalytic cofactor (2NZ4) as its best hit. Interestingly, 1MMS,C is not included in the top five of ARTS although when a search is done for 1MMS,C it finds 2GIS,A as a similar structure.

Table S9. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1MFQ,A. See legend for Table S1.

	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1MFQ, A  **Molecule:** 7S RNA of human signal recognition particle (SRP) **Graph Topology :** 9_19   1MFQ	**1)** 1z43:A 7S.S SRP RNA **Score**= 60 **RMSD**= 1.61 **Graph Topology:** 7_3  **2)** 2hgu:A 23S rRNA **Score**= 59 **RMSD**= 1.81 **Graph Topology:** N/A  **3)** 1vqm:40 23S rRNA **Score**= 58 **RMSD**= 1.95 **Graph Topology:** N/A  **4)** 1yl4:A1 16S rRNA-mRNA **Score**= 57 **RMSD**= 1.78 **Graph Topology:** N/A	**1)** 1RY1, A ALU DOMAIN (SRP9, SRP14 + RNA) **E-value**= 4.00E-84 **RMSD**= 0.001 **Graph Topology:** 9_19  **2)** 2J37, A SRP RNA **E-value**= 4.00E-84 **RMSD**= 0.001 **Graph Topology:** 9_19  **3)** 2GO5, A SRP RNA **E-value**= 1.00E-79 **RMSD**= 3.304 **Graph Topology:** 9_19  **4)** 4P3E, A SRP RNA **E-value**= 7.00E-12 **RMSD**= 1.484 **Graph Topology:** 7_3	**Subgraph ID 9_19:** **1)** 2J37, A SRP RNA **RMSD**= 0.003 **Graph Topology:** 9_19  **2)** 2GO5, A SRP RNA **RMSD**= 2.262 **Graph Topology:** 9_19  **Subgraph ID 8_10 (A):** **1)** 2J37, A SRP RNA **RMSD**= 0.003 **Graph Topology:** 9_19  **2)** 2GO5, A SRP RNA **RMSD**= 2.849 **Graph Topology:** 9_19  **3)** 1L9A, B SRP RNA **RMSD**= 4.904



5) 2nz4:FQ
GlmS ribozyme-substrate
Score= 56
RMSD= 1.88
Graph Topology: 6_5



5) 3KTV, C
SRP RNA
E-value= 5.00E-10
RMSD= 1.832
Graph Topology: 7_3

Graph Topology: 9_19

Subgraph ID 8_10 (B):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 2.849
Graph Topology: 9_19

3) 1L9A, B
SRP RNA
RMSD= 5.215
Graph Topology: 9_19

Subgraph ID 8_5:
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 1.292
Graph Topology: 9_19

3) 1L9A, B
SRP RNA
RMSD= 3.474
Graph Topology: 9_19

Subgraph ID 7_8:
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 2.171
Graph Topology: 9_19

3) 1L9A, B
SRP RNA
RMSD= 4.904
Graph Topology: 9_19

Subgraph ID 7_3 (A):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 2.463
Graph Topology: 9_19

Subgraph ID 7_3 (B):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 2.271
Graph Topology: 9_19

Subgraph ID 7_3 (C):
1) 2J37, A

SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 1.322
Graph Topology: 9_19

Subgraph ID 7_3 (D):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 1.349
Graph Topology: 9_19

Subgraph ID 6_3 (A):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 2.180
Graph Topology: 9_19

Subgraph ID 6_3 (B):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 2.128
Graph Topology: 9_19

Subgraph ID 6_3 (C):
1) 2J37, A
SRP RNA
RMSD= 0.002
Graph Topology: 9_19

2) 2GO5, A
SRP RNA

RMSD= 1.800
Graph Topology: 9_19

Subgraph ID 6_2 (A):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 1.866
Graph Topology: 9_19

Subgraph ID 6_2 (B):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2) 2GO5, A
SRP RNA
RMSD= 2.012
Graph Topology: 9_19

Subgraph ID 5_2 (A):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

2)2GO5, A
SRP RNA
RMSD= 2.530
Graph Topology: 9_19

Subgraph ID 5_2 (B):
1) 2J37, A
SRP RNA
RMSD= 0.002
Graph Topology: 9_19

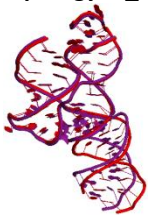
2)2GO5, A
SRP RNA
RMSD= 2.180
Graph Topology: 9_19

Subgraph ID 5_2 (C):
1) 2J37, A
SRP RNA
RMSD= 0.002
Graph Topology: 9_19

2)2GO5, A
SRP RNA
RMSD= 2.128
Graph Topology: 9_19

Subgraph ID 4_2:
1) 2J37, A
SRP RNA
RMSD= 0.002
Graph Topology: 9_19

2)2GO5, A
SRP RNA
RMSD= 1.605
Graph Topology: 9_19



Subgraph ID 3_1 (A):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

Subgraph ID 3_1 (B):
1) 2J37, A
SRP RNA

RMSD= 0.003
Graph Topology: 9_19

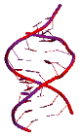
Subgraph ID 2_1 (A):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

Subgraph ID 2_1 (B):
1) 2J37, A
SRP RNA
RMSD= 0.002
Graph Topology: 9_19

Subgraph ID 2_1 (C):
1) 2J37, A
SRP RNA
RMSD= 0.003
Graph Topology: 9_19

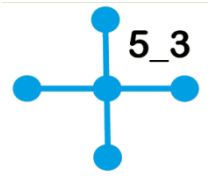
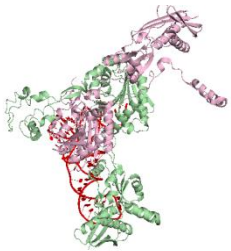
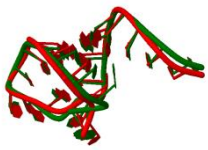
Subgraph ID 2_1 (D):
1) 2E9Z, BC
template- primer RNA
RMSD= 0.001
Graph Topology: 2_1

2) 4IQX, BC
template- primer RNA
RMSD= 0.022
Graph Topology: 2_1

			 **3)** 2E9R, AB template- primer RNA **RMSD**= 0.051 **Graph Topology:** 2_1  **4)** 3KLV, BC template- primer RNA **RMSD**= 0.067 **Graph Topology:** 2_1  **5)** 3KNA, BC template- primer RNA **RMSD**= 0.070 **Graph Topology:** 2_1  **Subgraph ID 2_1 (E):** **1)** 2J37, A SRP RNA **RMSD**= 0.405 **Graph Topology:** 9_19 

1MFQ is the structure of a human SRP ternary complex consisting of SRP19, the M domain of SRP54 and the S domain of 7SL RNA. Both R3D-Blast and RAG-3D return SRP RNAs from different ribosome-nascent-chain complexes (2J37,A and 2GO5,A). Interestingly, RAG-3D finds RNA matches from Foot-and-mouth disease virus RNA-polymerase complexes (2E9Z, 4IQX, 2E9R, 3KLV, 3KNA) in the results of 2_1 (D) topology ID. The best hit of ARTS, 1Z43,A, which is the structure of the S-domain of SRP RNA is also found by RAG-3D but listed in different rankings since it is a poor match due to large RMSD values. Interestingly, 1LNG,B is not included in the top five of ARTS although when a search is done for 1LNG,B it finds 1MFQ,A as a similar structure.

Table S10. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 2DU3,D. See legend for Table S1.

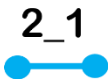
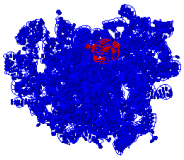
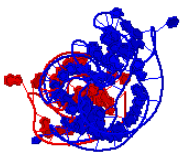
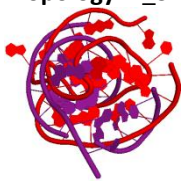
	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 2DU3, D  **Molecule:** tRNA **Graph Topology :** 5_3   2DU3	**1)** 2du6:D tRNA **Score**= 109 **RMSD**= 0.79 **Graph Topology:** 6_6  **2)** 1wz2:D tRNA **Score**= 85 **RMSD**= 1.71 **Graph Topology:** 6_6  **3)** 486d:C tRNA **Score**= 83 **RMSD**= 1.69 **Graph Topology:** 5_3  **4)** 2der:C tRNA **Score**= 80 **RMSD**= 1.83 **Graph Topology:** 4_2 	**1)** 2DU4, C tRNA **E-value**= 1.00E-40 **RMSD**= 0.636 **Graph Topology:** 5_3  **2)** 2DU5, D tRNA **E-value**= 5.00E-34 **RMSD**= 0.737 **Graph Topology:** 5_3  **3)** 2DU6, D tRNA **E-value**= 1.00E-28 **RMSD**= 0.818 **Graph Topology:** 5_3  **4)** 2XUY, V tRNA **E-value**= 3.00E-07 **RMSD**= 1.416 **Graph Topology:** 5_3 	**Subgraph ID 5_3:** **1)** 2DU6, D tRNA **RMSD**= 0.497 **Graph Topology:** 5_3  **2)** 2DU4_C tRNA **RMSD**= 0.869 **Graph Topology:** 5_3  **3)** 1IL2_D tRNA **RMSD**= 1.203 **Graph Topology:** 5_3  **4)** 2DU5_D tRNA **RMSD**= 1.321 **Graph Topology:** 5_3 

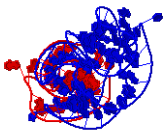
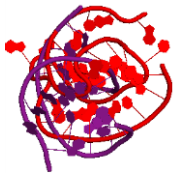
5) 2j02:W tRNA **Score**= 75 **RMSD**= 1.86 **Graph Topology:** 5_3 	**5)** 2CSX, D 75-mer RNA **E-value**= 4.00E-07 **RMSD**= 1.469 **Graph Topology:** 6_5 	**5)** 3J0V_B tRNA **RMSD**= 1.341 **Graph Topology:** 5_3 

2DU3 is a tRNA in complex with O-phosphoseryl-tRNA synthetase and contains a 4-way junction. All tools successfully find the same tRNA in complex with O-phosphoseryl-tRNA synthetase E418N/E420N mutant (2DU6). Both R3D-BLAST and RAG-3D also find the same tRNA from different complexes (2DU4,C , 2DU5,D). The third hit of RAG-3D is a tRNA in complex with aspartyl-tRNA synthetase, and the fifth hit of R3D-BLAST is a tRNA in complex with Methionyl-tRNA synthetase. RAG-3D only compares this structure with other structures with 5_3 topology since the junction must remain intact.

ARTS returns a tRNA in complex with Leucyl-tRNA synthetase (1WZ2,D) in the second, and A-site tRNA of 70S ribosome (486D,C) in the third positions.

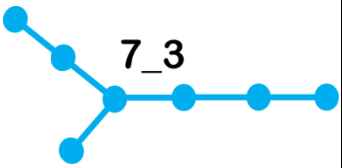
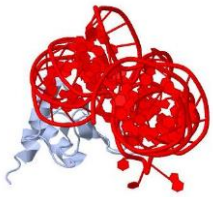
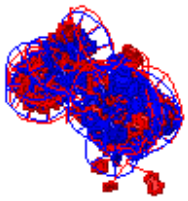
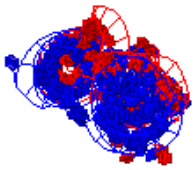
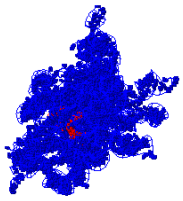
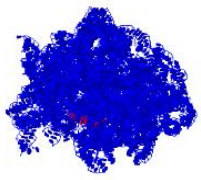
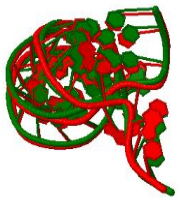
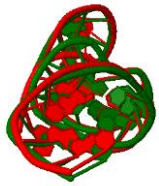
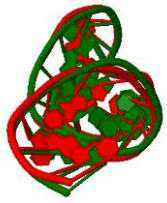
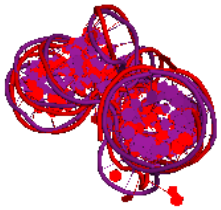
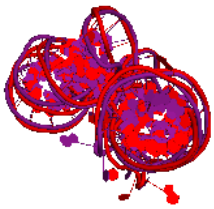
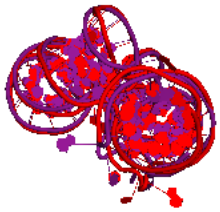
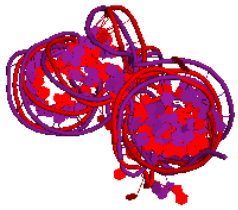
Table S11. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1L2X,A. See legend for Table S1.

	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1L2X, A  **Molecule:** Viral RNA Pseudoknot **Graph Topology :** 2_1   1L2X	**1)** 2i2v:B 23S rRNA **Score**= 30 **RMSD**= 1.75 **Graph Topology:** N/A  **2)** 1qf6:B tRNA **Score**= 29 **RMSD**= 1.58 **Graph Topology:** 5_3  **3)** 2i2u:A 16S rRNA **Score**= 29 **RMSD**= 1.92 **Graph Topology:** N/A  **4)** 1y26:X A-riboswitch-adenine complex **Score**= 28 **RMSD**= 1.63 **Graph Topology:** 4_2  **5)** 1u8d:A mRNA **Score**= 28 **RMSD**= 1.69	**1)** 437D, A RNA Pseudoknot **E-value**= 3.00E-15 **RMSD**= 0.58 **Graph Topology:** 2_1 	**Subgraph ID 2_1:** **1)** 3KNK, B 5S rRNA **RMSD**= 0.034 **Graph Topology:** 7_3  **2)** 3JYX, 4 5.8S rRNA **RMSD**= 0.042 **Graph Topology:** 3_1  **3)** 3IZT, A 50S rRNA 5S **RMSD**= 0.043 **Graph Topology:** 7_3  **4)** 3ZEX, D 5S rRNA **RMSD**= 0.048 **Graph Topology:** 8_5  **5)** 4A1C, 3 5S rRNA **RMSD**= 0.092 **Graph Topology:** 8_5

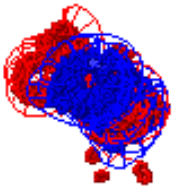
Graph Topology: 4_2		
		

We see no similarities among results of the viral RNA pseudoknot 1L2X,A from beet western yellow virus. R3D-Blast returns only one similar RNA pseudoknot structure, 437D,A from beet western yellow virus which is also found by RAG-3D in position nine. RAG-3D also finds many similar 2_1 substructures such as 5S rRNAs, and 5.8S rRNAs from different larger structures. Two of the results returned by ARTS have more than 10 vertices which are not included in the RAG database, and the other results are of 5_3 and 4_2 topologies which have no subgraphs due to junction intactness.

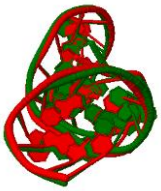
Table S12. Comparison of RAG-3D results to those for ARTS and R3D-BLAST and RAG-3D for 1LNG,B. See legend for Table S1.

	ARTS	R3D-BLAST	RAG-3D
PDB ID, Chain ID: 1LNG, B  **Molecule:** 7S.S signal recognition particle (SRP) RNA of SRP19 RNA complex **Graph Topology :** 7_3   1LNG	**1)** 1z43:A 7S.S SRP RNA **Score**= 158 **RMSD**= 1.44 **Graph Topology:** 7_3  **2)** 1mfq:A SRP RNA **Score**= 66 **RMSD**= 1.87 **Graph Topology:** 9_19  **3)** 1yl4:A1 16S rRNA-mRNA **Score**= 63 **RMSD**= 1.87 **Graph Topology:** N/A  **4)** 1vqm:40 23S rRNA **Score**= 59 **RMSD**= 1.69 **Graph Topology:** N/A 	**1)** 2V3C, N 7S.S SRP RNA **E-value**= 4.00E-07 **RMSD**= 1.02 **Graph Topology:** 7_3  **2)** 2V3C, M 7S.S SRP RNA **E-value**= 4.00E-05 **RMSD**= 1.254 **Graph Topology:** 7_3  **3)** 2V3C, N 7S.S SRP RNA **E-value**= 0.002 **RMSD**= 1.199 **Graph Topology:** 7_3  **4)** 2V3C, M 7S.S SRP RNA **E-value**= 0.004 **RMSD**= 1.198 **Graph Topology:** 7_3 	**Subgraph ID 7_3:** **1)** 1Z43, A 7S.S SRP RNA **RMSD**=1.023 **Graph Topology:** 7_3  **2)** 2V3C, M 7S.S SRP RNA **RMSD**=1.078 **Graph Topology:** 7_3  **3)** 2V3C, N 7S.S SRP RNA **RMSD**=1.169 **Graph Topology:** 7_3  **4)** 3KTW, C SRP RNA **RMSD**=2.488 **Graph Topology:** 7_3 

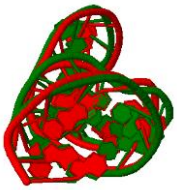
5) 2d1b:AB
39-mer RNA
Score= 59
RMSD= 1.90
Graph Topology: 4_1



5) 3NDB, M
7S.S SRP RNA
E-value= 0.008
RMSD= 1.029
Graph Topology: 8_10

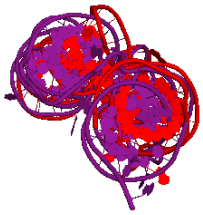


6) 1Z43, A
7S.S SRP RNA
E-value= 0.008
RMSD= 1.144
Graph Topology: 7_3

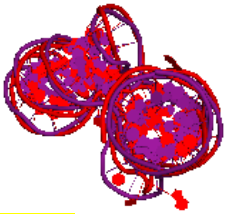


7) 3LQX, B
SRP RNA
E-value= 0.008
RMSD= 1.525
Graph Topology: 4_1

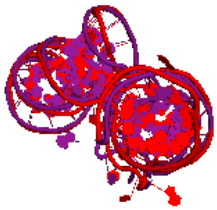
5) 3KTV, A
SRP RNA
RMSD=3.754
Graph Topology: 7_3



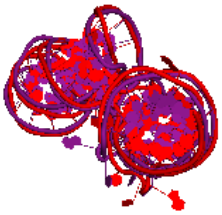
Subgraph ID 6_3:
1) 1Z43, A
7S.S SRP RNA
RMSD=1.029
Graph Topology: 7_3



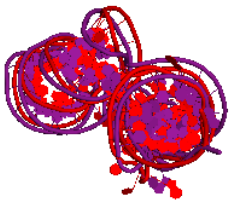
2) 2V3C, N
7S.S SRP RNA
RMSD=1.039
Graph Topology: 7_3



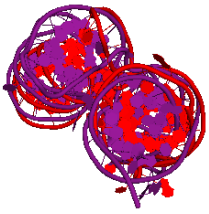
3) 2V3C, M
7S.S SRP RNA
RMSD=1.058
Graph Topology: 7_3



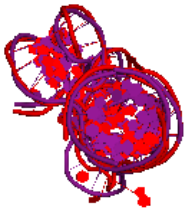
4) 3KTW, C
SRP RNA
RMSD=2.885
Graph Topology: 7_3



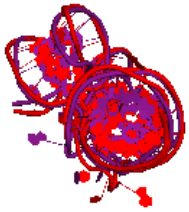
5) 3KTV, A
SRP RNA
RMSD=3.696
Graph Topology: 7_3



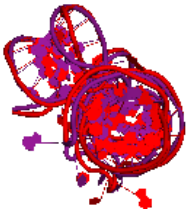
Subgraph ID 6_2:
1)) 1Z43, A
7S.S SRP RNA
RMSD=0.956
Graph Topology: 7_3



2) 2V3C, M
7S.S SRP RNA
RMSD=1.099
Graph Topology: 7_3

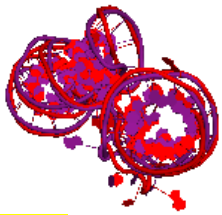


3) 2V3C, N
7S.S SRP RNA
RMSD=1.391
Graph Topology: 7_3

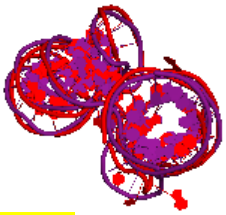


Subgraph ID 5_2 (A):
1) 2V3C, M
7S.S SRP RNA

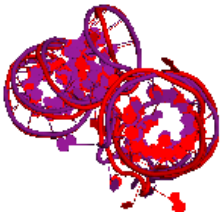
RMSD=1.007
Graph Topology: 7_3



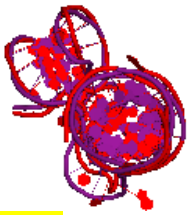
2) 1Z43, A
7S.S SRP RNA
RMSD=1.080
Graph Topology: 7_3



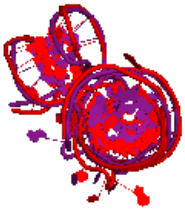
3) 2V3C, N
7S.S SRP RNA
RMSD=1.267
Graph Topology: 7_3



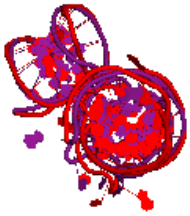
Subgraph ID 5_2 (B):
1) 1Z43, A
7S.S SRP RNA
RMSD=0.921
Graph Topology: 7_3



2) 2V3C, M
7S.S SRP RNA
RMSD=1.014
Graph Topology: 7_3



3) 2V3C, N
7S.S SRP RNA
RMSD=1.236
Graph Topology: 7_3



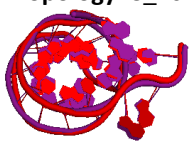
Subgraph ID 4_2:
1) 2V3C, M
7S.S SRP RNA
RMSD=0.937
Graph Topology: 7_3

2) 1Z43, A
7S.S SRP RNA
RMSD=0.945
Graph Topology: 7_3

Subgraph ID 3_1:
1) 1Z43, A
7S.S SRP RNA
RMSD=0.631
Graph Topology: 7_3

2) 1QZW, B
7S SRP RNA
RMSD=0.720
Graph Topology: 4_1

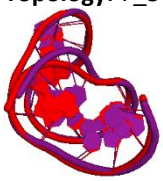
Subgraph ID 2_1 (A):
1) 3NDB, M
SRP RNA
RMSD=0.378
Graph Topology: 8_10



Subgraph ID 2_1 (B):
1) 1ZE2, C
22-mer RNA
RMSD=0.009
Graph Topology: 2_1

2) 1P6V, D
45-mer RNA
RMSD=0.030
Graph Topology: 2_1

Subgraph ID 2_1 (C):
1) 2V3C, M
7S.S SRP RNA
RMSD=0.334
Graph Topology: 7_3



All three tools return the 7S.S signal recognition particle (SRP) RNA 1Z43,A as a matching result. ARTS and RAG-3D find 1Z43,A ranked first, and R3D-Blast ranked sixth. It is interesting that RAG-3D finds matching 7_3 motifs from a SRP19/S-domain SRP RNA complex, 3KTV,A and 3KTW,A that are found by neither ARTS nor R3D-Blast. The 7S RNA motifs 2V3C,M and 2V3C,N of the large SRP54-SRP19-7S.S SRP RNA complex are successfully returned by both R3D-Blast and RAG-3D. The other SRP RNA hits returned by R3D-Blast are also found by RAG-3D but in higher orders due to larger RMSD values. The fifth result of RAG-3D in 7_3 matching list, 3KTW,C, is interesting since it shares a 3-way junction with the query. Furthermore, RAG-3D identifies similar 2_1 motifs such as a SRP RNA bound to a signaling protein (3NDB,M), a tRNA in complex with Pseudouridine synthase protein (1ZE2,C) and tRNA-like domain of tmRNA that combines the functions of both transfer and messenger RNAs in complex with small protein B (1P6V, D).

Table S13. Comparison of run time in seconds

PDB ID, Chain ID	Molecule	Graph Topology	Number of Subgraphs	Run time (s)		
				ARTS	R3D-BLAST	RAG-3D
1E8O_E	7SL RNA	4_2	1	39	4.3	4.0
3F30_X	FMN Riboswitch	8_18	1	40	15.2	2.7
1ASY_R	tRNA	5_3	1	31.2	13.7	3.8
1C04_E	23S rRNA fr	5_2	3	24.8	16.5	16.5
2CSX_D	Ligase/RNA	6_5	3	36.4	13.8	13.5
2GIS_A	SAM-I Riboswitch	7_7	6	41.5	15.1	24.8
3IYR_A	tmRNA	10_61	6	18.4	11.3	16.1
3J62_B	5S rRNA	7_3	10	39.9	16.3	45.6
4KQY_A	SAM-I Riboswitch	8_2	14	42.4	6.4	43.8
2R8S_R	Ribozyme	10_2	24	48.5	16.8	56.8