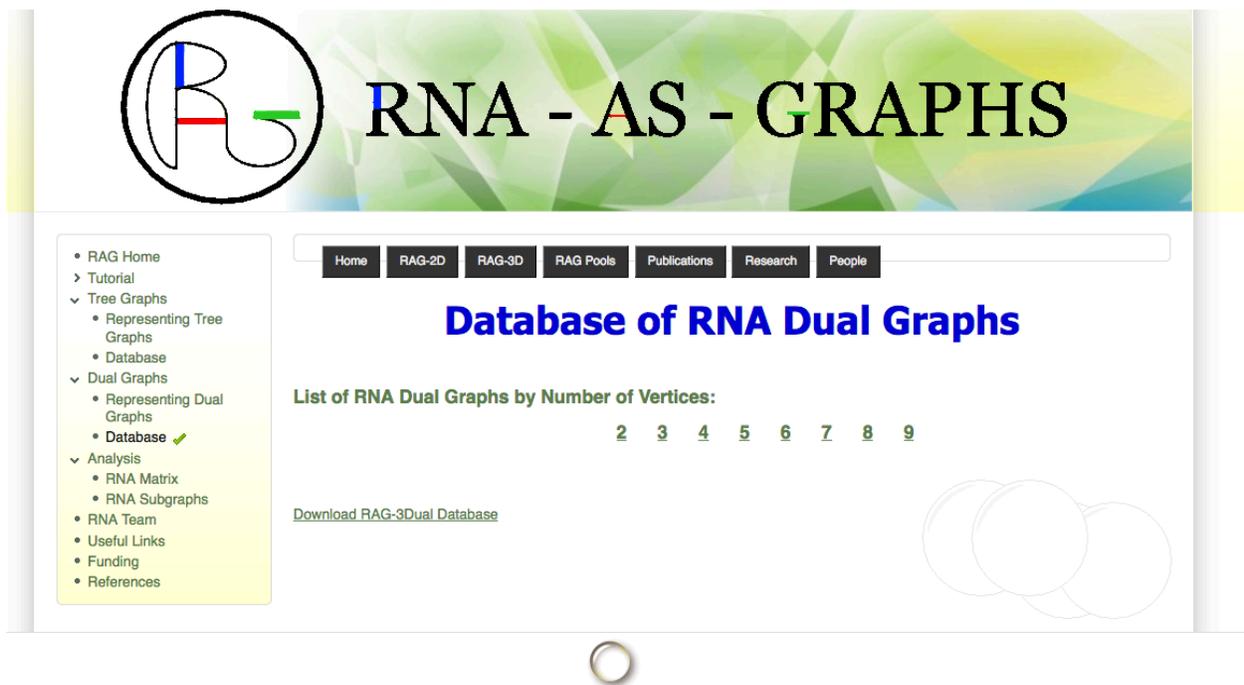


## The Schlick lab RNA-As-Graphs Dual Graph Resource

Our dual graph resource (available at: [http://www.biomath.nyu.edu/?q=rag/dual\\_vertices.php](http://www.biomath.nyu.edu/?q=rag/dual_vertices.php)) consists of two parts as shown in Figure 1:

The first part lists the 94 dual graph topologies between 2-9 vertices that correspond to existing RNA structures in the representative RNA dataset. All existing dual graph topologies are shown on the corresponding vertex page. For example, Figure 2 shows the 6 existing dual graph topologies with 3 vertices. RNA structures and chains from the representative dataset corresponding to each existing dual graph topology are also listed. For example, Figure 3 shows the list of 8 RNA PDB files and chains that correspond to the dual graph topology 3\_2.

The second part contains the link to download the *RAG-3Dual database* (as a single zipped file), that contains the non-separable subgraph blocks and corresponding RNA atomic fragments. These non-separable blocks are obtained by applying dual graph partitioning to the 2D structures in the representative RNA dataset ( $\geq 2$  vertices). The atomic fragments are cataloged based on their dual graph IDs.



The screenshot shows the homepage of the RNA-As-Graphs resource. At the top left is a logo consisting of a circle with a stylized 'R' and 'S' inside, colored in blue, red, and green. To the right of the logo, the text 'RNA - AS - GRAPHS' is displayed in a large, bold, black serif font. Below the logo and title is a navigation bar with buttons for 'Home', 'RAG-2D', 'RAG-3D', 'RAG Pools', 'Publications', 'Research', and 'People'. The main heading is 'Database of RNA Dual Graphs' in a bold blue font. Below this is a section titled 'List of RNA Dual Graphs by Number of Vertices:' with a horizontal list of numbers from 2 to 9, each in a different color. A link 'Download RAG-3Dual Database' is visible below the list. On the left side, there is a sidebar menu with a tree structure of links, including 'RAG Home', 'Tutorial', 'Tree Graphs', 'Dual Graphs', 'Analysis', and 'References'. The 'Database' link under 'Dual Graphs' is highlighted with a green checkmark. At the bottom center of the page, there is a small circular icon.

Figure 1: Two parts of our dual graph resource.

- RAG Home
- > Tutorial
- ✓ Tree Graphs
  - Representing Tree Graphs
  - Database
- ✓ Dual Graphs
  - Representing Dual Graphs
  - Database ✓
- ✓ Analysis
  - RNA Matrix
  - RNA Subgraphs
  - RNA Team
  - Useful Links
  - Funding
  - References

# Database of RNA Dual Graphs

## List of RNA Dual Graphs by Number of Vertices:

[2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#)

[Download RAG-3Dual Database](#)

### 3 VERTICES

Number of Possible RNA Topologies: 8  
 Number of Motifs Found: 6  
 Number of Missing Motifs: 2

To learn more about an RNA topology, please click on its graph.

These graphs have been ordered according to the second smallest eigenvalue of their Laplacian matrix ( $\lambda_2$  is given).

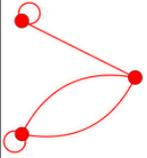
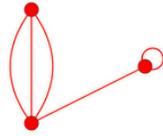
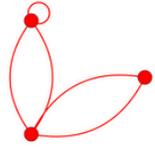
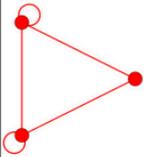
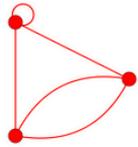
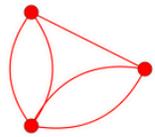
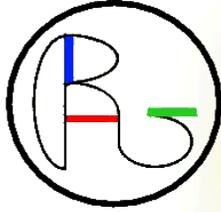
|                                                                                                                                   |                                                                                                                                   |                                                                                                                                     |
|-----------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| $\lambda_2$<br>ID: (3_2)<br>= 1.2679492235<br>  | $\lambda_2$<br>ID: (3_3)<br>= 1.3542486429<br>  | $\lambda_2$<br>ID: (3_4)<br>= 2.0000000000<br>  |
| $\lambda_2$<br>ID: (3_5)<br>= 3.0000000000<br> | $\lambda_2$<br>ID: (3_6)<br>= 3.0000000000<br> | $\lambda_2$<br>ID: (3_8)<br>= 4.0000000000<br> |

Figure 2: The 6 existing dual graph topologies with 3 vertices.

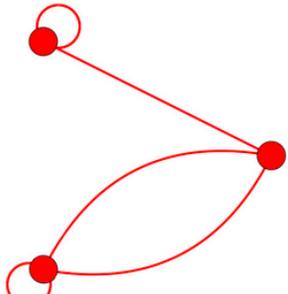


# RNA - AS - GRAPHS

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## Dual Topology: 3\_2



### Topological Aspects

- 3 Vertices
- Eigenvalues  
0.000000000  
1.2679492235  
4.7320508957

Examples of actual RNAs corresponding to this structure from RNA databases: 8

| PDB_Chain | Type                                      | Discovery Method    |
|-----------|-------------------------------------------|---------------------|
| 1M5K_E    | RNA HAIRPIN RIBOZYME                      | X-RAY DIFFRACTION   |
| 3IZZ_A    | Helix 5, 14, 15 (Small Subunit)           | ELECTRON MICROSCOPY |
| 3J0D_A    | ribosomal 23S RNA                         | ELECTRON MICROSCOPY |
| 3JCT_6    | ITS2-1 miscRNA                            | ELECTRON MICROSCOPY |
| 4PKD_V    | U1 snRNA stem-loops 1 and 2 (55-MER)      | X-RAY DIFFRACTION   |
| 4WZJ_YYYY | U4 small nuclear RNA variant              | X-RAY DIFFRACTION   |
| 5CZZ_B    | RNA (73-MER)                              | X-RAY DIFFRACTION   |
| 5WSG_E    | Saccharomyces cerevisiae S288c SNR6 snRNA | ELECTRON MICROSCOPY |

Figure 3: List of RNA PDB files and chains corresponding to the existing dual graph topology 3\_2.