



RinPy – Residue Interaction Network for Protein Structures

RinPy User Graphical Interface (GUI)

User Manual (v0.1.0)

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1 Introduction

RinPy, a pip-installable open-source Python package, is designed for constructing, visualizing, and analyzing Residue Interaction Networks (RINs). RIN describes a protein as a network of nodes interconnected by weighted edges. In this network, each node represents a residue, nucleotide or a ligand at the average coordinate of its atomic coordinates. The edge weight between two nodes is defined by the local interaction strength between the two residues. The average coordinates of the residues and/or nucleotides are placed at the *C_α* atom or P atom, respectively, for the protein-RNA/DNA complexes. Each node is annotated with attributes such as Chain ID, Residue Number, Insertion Code, and its Cartesian coordinates. To facilitate ease of use, the RinPy GUI application was developed as a companion to this package, with a user-friendly design intended for the scientific community.

Figure 1 illustrates the main components of the RinPy GUI application. The interface consists of four core components as follows:

- ✓ **Input and output selection**, which supports directories containing PDB files, direct PDB ID input, and snapshot PDB files that include multiple frames extracted from an MD trajectory (see Section 3 for details).
- ✓ **Parameter configuration**, including heteroatom selection, for generating residue interaction networks from the selected protein structures (see Section 4 for details).
- ✓ **Process monitoring**, which displays the real-time status of the running analysis (see Section 5 for details).
- ✓ **Execution and logging**, allowing users to initiate the RIN generation process and optionally download the corresponding execution logs (see Section 6 for details).

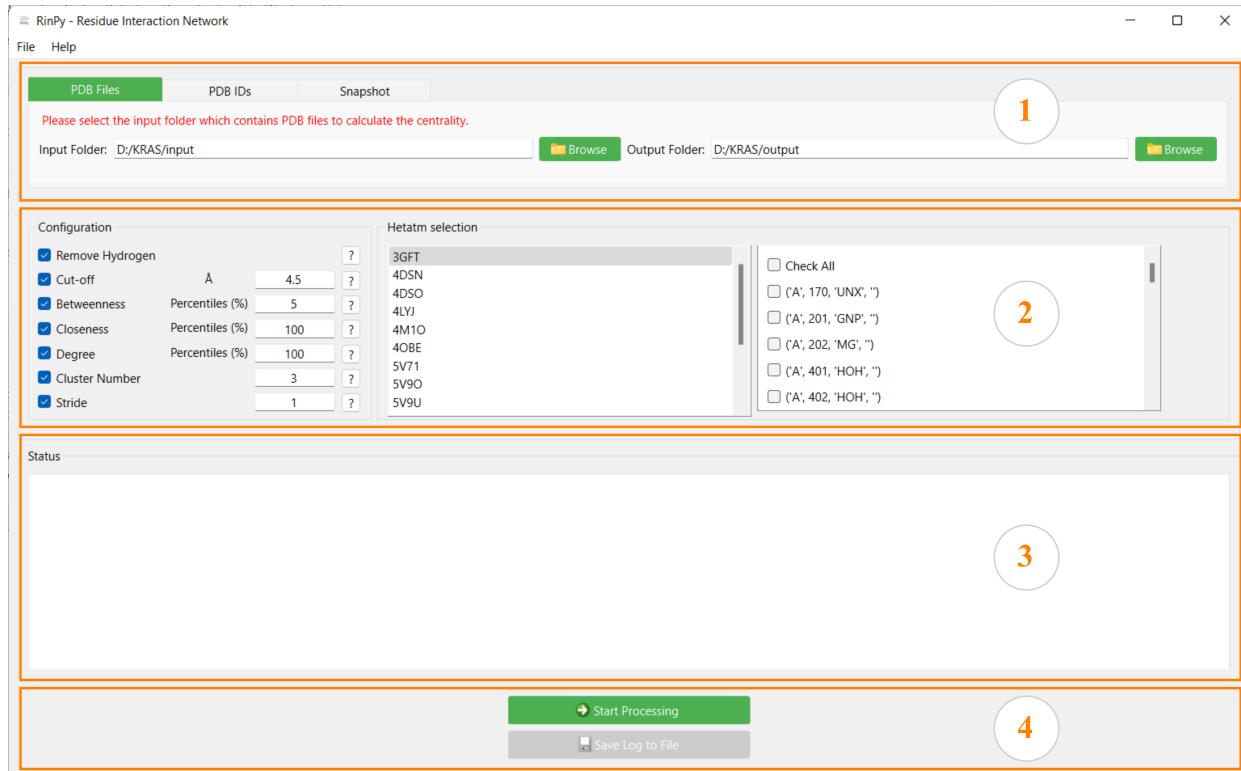


Figure 1: Overview of the RinPy GUI application highlighting its main interface components.

2 Menu Items

The RinPy GUI application includes two main menus: **File** and **Help**. The **File** menu provides an **Exit** option that allows users to close the application. The **Help** menu contains **User Manual** and **About** options. Through the **User Manual** option, users can view and download the documentation, which provides detailed instructions on how to use the application. The **About** option presents general information about the application, including its purpose, version, and related details. Figure 2 highlights each of these menu options.

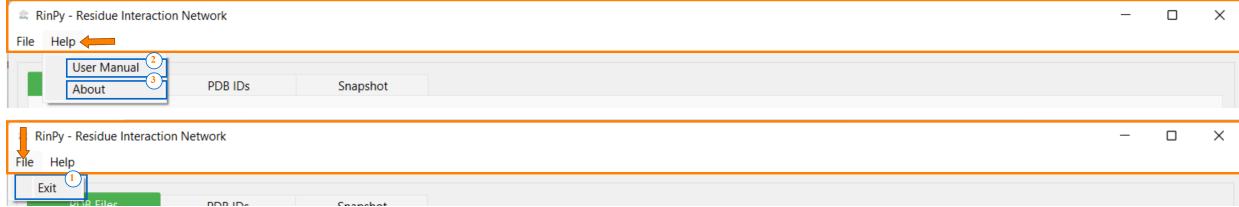


Figure 2: Details of the main menu and its action options.

3 Input/Output Selection

The RinPy GUI offers several methods for loading input structures, together with output directory selection:

- ✓ Selecting a folder containing one or more PDB files from the workspace (Figure 3).
- ✓ Fetching structures directly from the Protein Data Bank (rcsb.org) by entering PDB IDs. After specifying the output folder, users should click the **Download** button to initiate the retrieval process. The selected PDB files will be downloaded to the designated output folder for further processing (Figure 4).
- ✓ Loading a single PDB file that includes multiple snapshots extracted from an MD trajectory (Figure 5).

Note: Only one input option can be selected at a time. For all input methods, users must specify an output folder where the generated results will be saved.

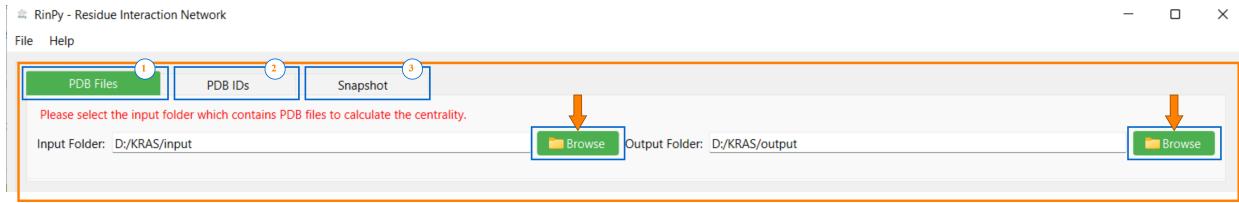


Figure 3: Input and output selection using the PDB Files tab as an example.

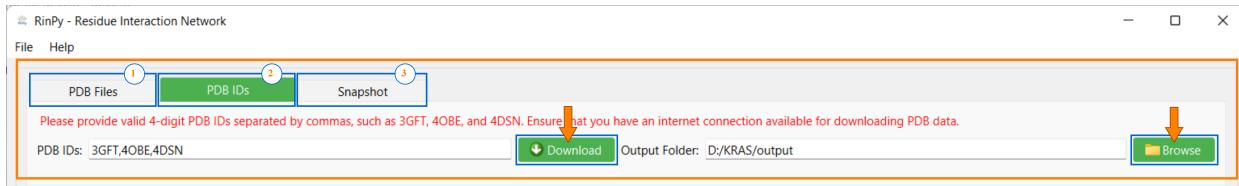


Figure 4: Input and output selection using the PDB IDs tab for retrieving structures from the Protein Data Bank.

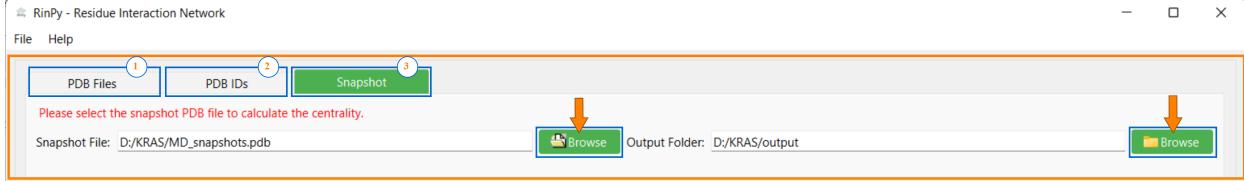


Figure 5: Input and output selection using the Snapshot tab for loading a PDB file containing multiple frames extracted from an MD trajectory.

4 Configuration Parameters

Figure 6 presents the configuration parameters that allow users to define the network generation settings in advance. A question mark icon next to each parameter provides a brief hint when hovered over with the mouse. When clicked, it opens a dialog box displaying detailed information about the corresponding parameter. Detailed descriptions of each parameter are provided in Table 1.

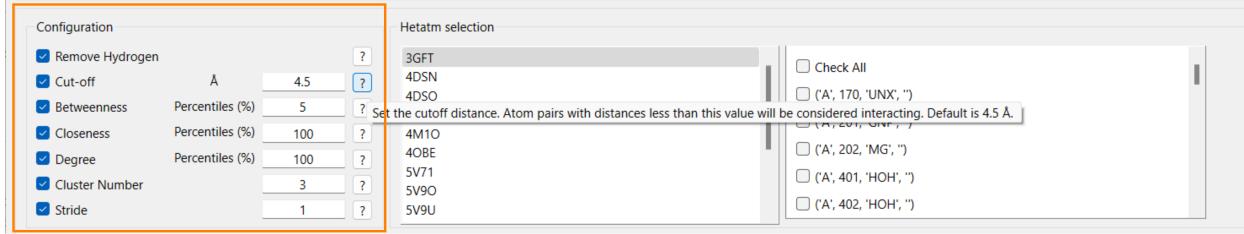


Figure 6: Configuration parameters used for generating residue interaction networks.

Table 1: User-defined selectable configuration parameters for residue interaction network generation.

Parameter	Detail	Selected	Default value
Remove Hydrogen	Remove Hydrogens.	True	True
Cut-off	The total number of heavy atom–atom distances between the corresponding residues within a specified cut-off distance. The default is 4.5 Å.	True	4.5 Å
Betweenness	Defines the percentage of residues with the highest betweenness centrality scores to be selected.	True	5%
Closeness	Defines the percentage of residues with the highest closeness centrality scores to be selected.	False	-
Degree	Defines the percentage of residues with the highest degree centrality scores to be selected.	False	-
Cluster number	Cluster number for graph spectral analysis, including hinges.	True	4
Stride	The step used to extract individual PDB structures from a PDB file containing MD trajectory snapshots.	True	1

Figure 7 shows the heteroatom selection options, allowing users to include nucleotides, cofactors, ligands, solvents, and crystallographic water molecules in the residue interaction network.

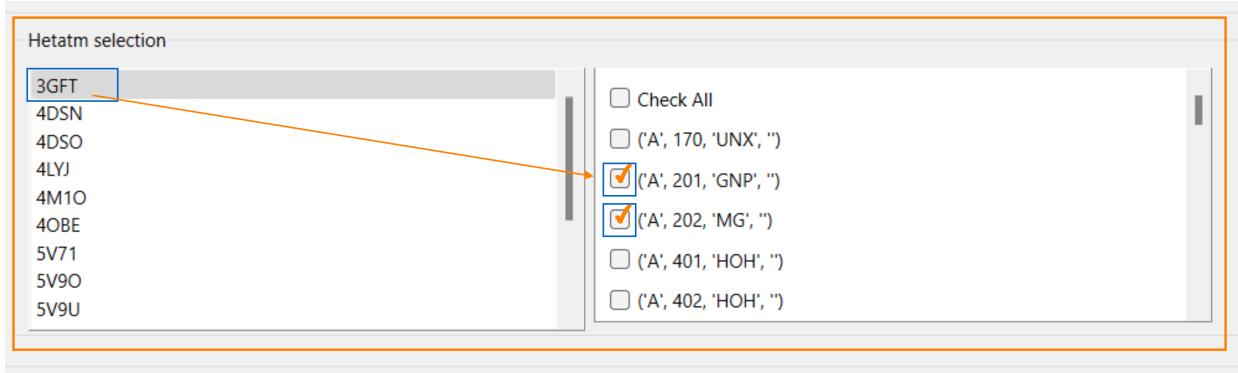


Figure 7: Heteroatom selection to be included in the generated residue interaction network.

5 Real-Time Monitoring of Process Status

The status panel displays real-time information about the execution process, such as the current analysis step and elapsed execution time, enabling users to monitor the progress of the computation (see Figure 8).

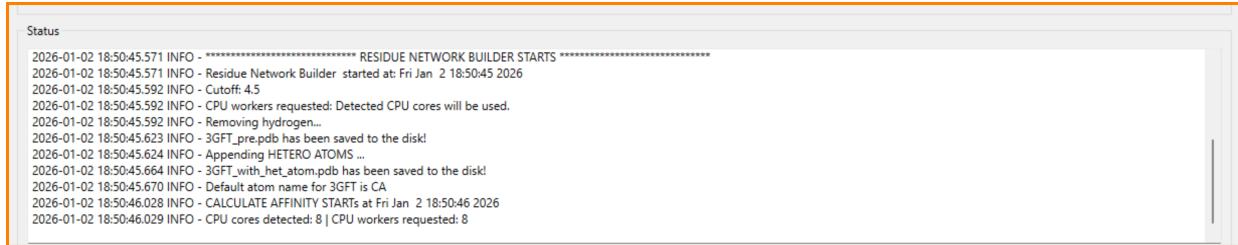


Figure 8: Status panel showing real-time execution progress and elapsed time.

6 Initiate RIN Process and Save Logs

Here, two action buttons are provided to manage the RIN generation process. The **Start Processing** button initiates the analysis for the selected input files once all input/output selections and configuration parameters are set. After the process is completed, the **Save Log to File** button allows users to export the entire process log to any directory of their choice for review. Also, the logs are automatically stored in the chosen output folder.

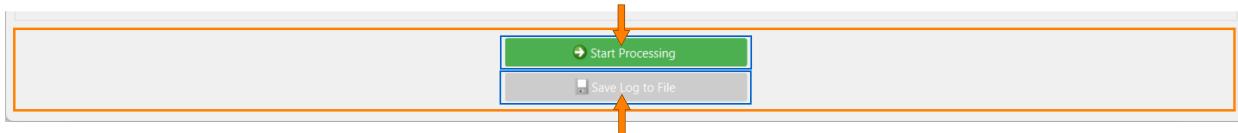


Figure 9: Action buttons for starting the process and saving process logs.

7 Usefull Links

The RinPy package used by the RinPy GUI application is available on PyPI [rinpy](https://pypi.org/project/rinpy/) and can be installed using **pip**.

The source code of the RinPy package is also publicly available on <https://github.com/kurkcuogluveitaslab/rinpy> and <https://github.com/zehrasarica/rinpy>.