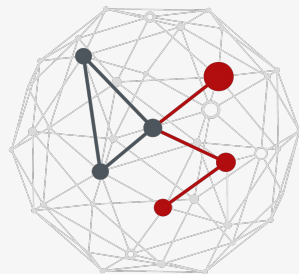


# Residue Interaction Network Generator (RING)

*Computer Science - Structural Bioinformatics*

2020





**DATA SCIENCE**  
UNIVERSITY OF PADOVA

# **Residue Interaction Network Generator - RING -**

Master of Science in Data Science

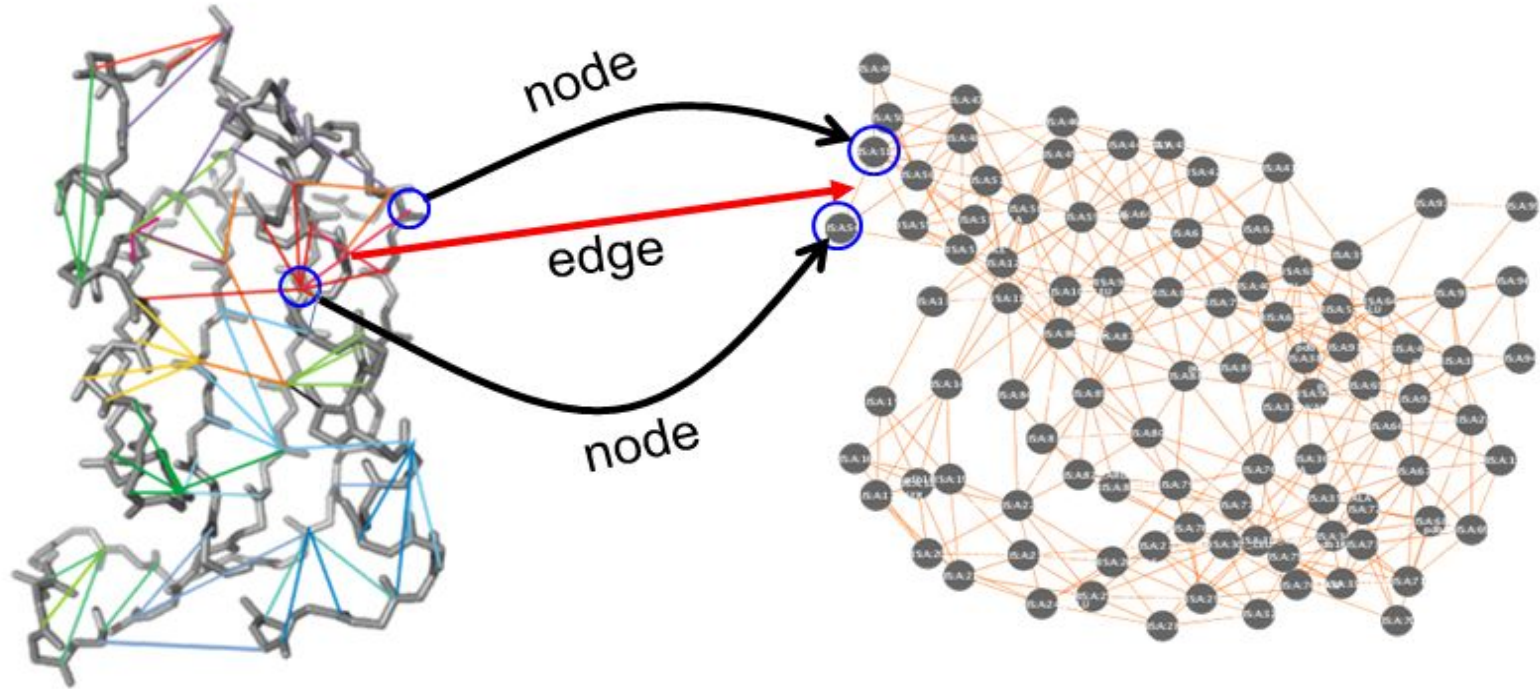
**Damiano Piovesan**



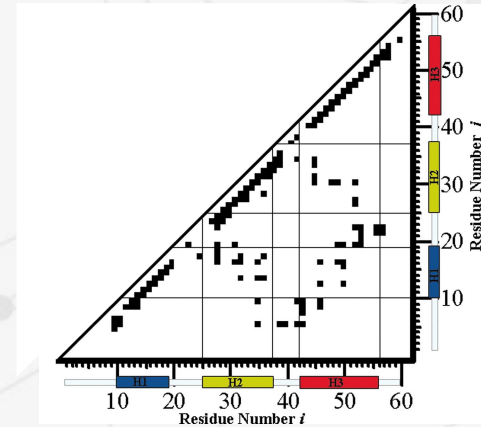
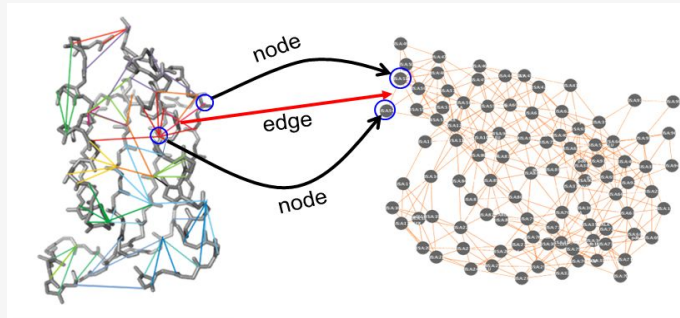
# Concept

3D coordinates (PDB)

Contacts (Graph)



# RIN and contact maps



## Why RINs?

- Functional features
- Effect of mutations
- Protein folding
- Intra protein domain–domain communication
- Catalytic activity
- Machine learning features (ex. contact maps)
- Molecular Dynamics Analysis

## RIN generator software

- PIC (2007)
- **RING (2011 – first release)**
- RINerator/RINalyzer (2014)
- NAPS (2016)



# Web server




# Residue Interaction Network Generator

The **Residue Interaction Network Generator (RING)** identifies **non-covalent interactions** at atomic level in protein structures. RING can process multi-state structures, including **molecular dynamics and structural ensembles**. It generates **probabilistic networks**, **conformational-dependent contact maps** and it is extremely **fast** scaling linearly with input size. The result page provides a synchronized and interactive side-by-side view of the network and structure. You can also **login** and save your analysis for a later use.

For questions and comments, please [contact us](#). RING output can also be generated with the [RING standalone package](#) (available as pre-build for Unix and MacOS systems).



### Job description

Example: Test with open conformation

PDB ID \*

Examples: [2H9R](#) [1K47](#) [2LP9](#)

Chain (all if empty)

Sequence separation \*

#### Nodes

☒ Closest  
 ☐ Lollipop  
 ☐ Cα  
 ☐ Cβ

#### Distance thresholds

☒ Strict  
 ☐ Relaxed  
 ☐ Manual

Hydrogen bond	<input type="text" value="3.5"/>	<input type="text" value="4"/>	ionic (salt bridge)	<input type="text" value="4"/>	<input type="text" value="5"/>
Van der Waals	<input type="text" value="0.5"/>	<input type="text" value="0.5"/>	π-π stacking	<input type="text" value="4"/>	<input type="text" value="5"/>
			Disulphide bond	<input type="text" value="2.5"/>	<input type="text" value="4"/>

#### Edges

☒ Multiple  
 ☐ All  
 ☐ One

#### Other options

☐ Skip hetero  
 ☐ Include water  
 ☐ Calculate energy

[Submit](#) [Reset](#)

\* Required fields

For very large molecular dynamics simulations (>500 models) or huge structures (>200 MB) please consider using the RING standalone package. You can find more information on how RING works in the [about](#) page. A brief overview and a description of the inputs, outputs and available APIs is available in the [help](#) page.

**RING 3.0: fast generation of probabilistic residue interaction networks from structural ensembles**

Damiano Clemente, Alessio Del Conte, Alexander Miguel Monzon, Gloria F. Camagni, Giovanni Minervini, Damiano Piovesan and Silvio C.E. Tosatto

(2022) [Nucleic Acids Research](#), accepted for publication [DOI](#)

RING created by BioComputing UP lab, University of Padua, Italy



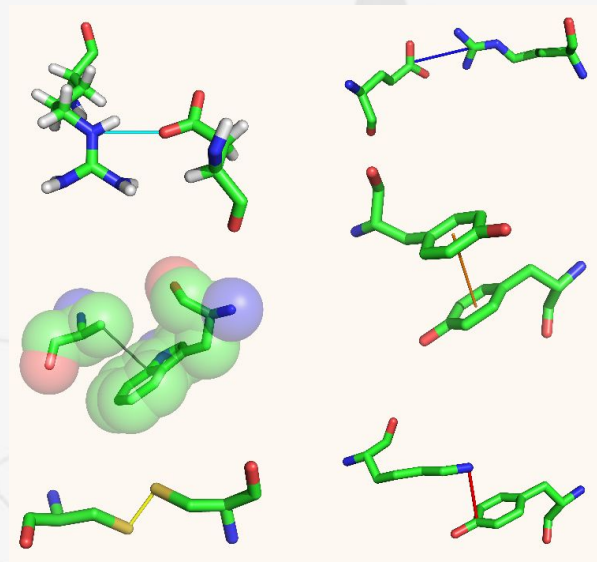
<https://ring.biocomputingup.it>

*RING 3.0: fast generation of probabilistic residue interaction networks from structural ensembles.*  
Clementel et al., **NAR**, 2022, 44(W1), W367–W374



# Types of interactions

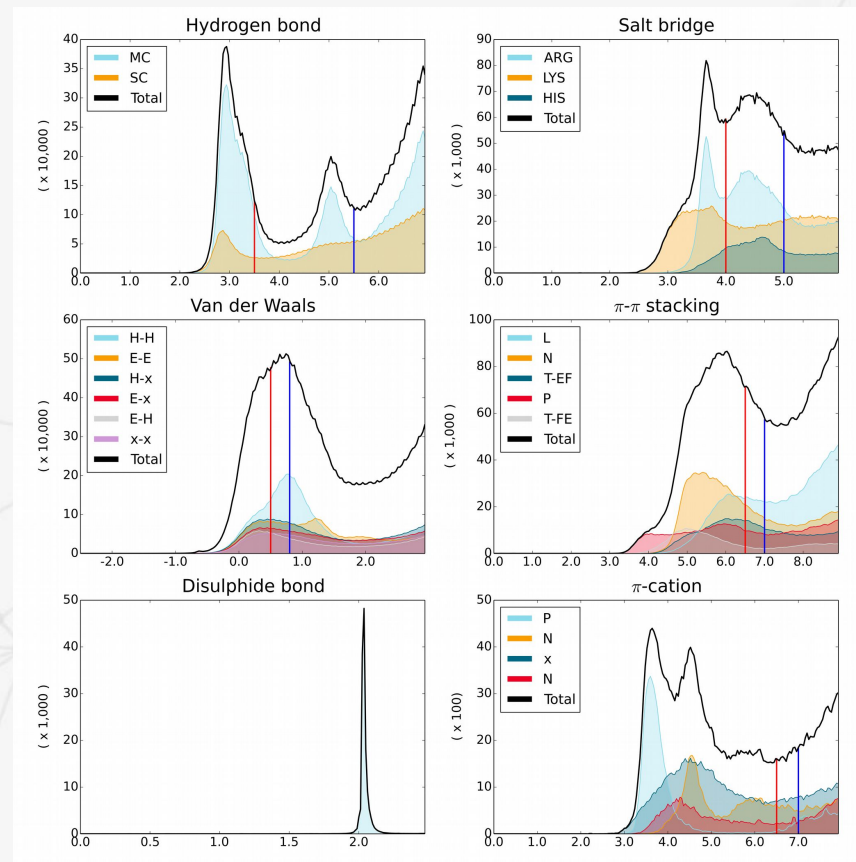
- **Hydrogen bond (HBOND)**
- **Van der Waals interactions (VDW)**
- **Disulfide bridges (SBOND)**
- **Salt bridges (IONIC)**
- **$\pi$ - $\pi$  stacking (PIPISTACK)**
- **$\pi$ -cation (PICATION)**
- **Inter-Atomic Contact (IAC)**, close residues but untyped interaction



# Distance cutoff

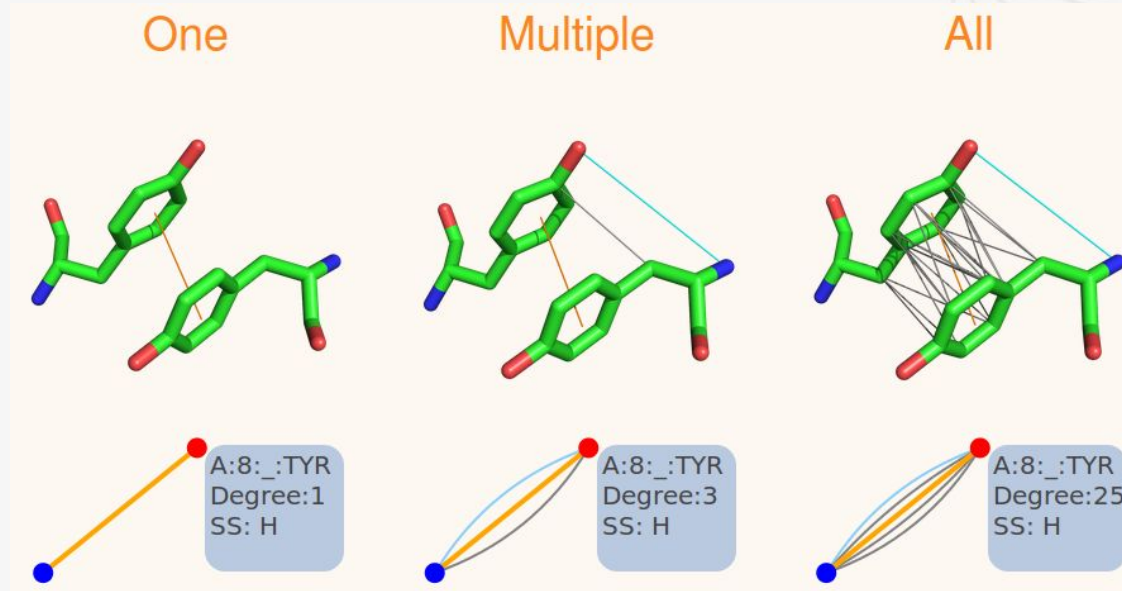
- Relaxed
- Strict (default)

*The RING-2.0 web server for high quality residue interaction networks.* Piovesan D, Minervini G, Tosatto, SCE. **NAR**, 2016, 44(W1), W367-74





# Number of interactions per residue



# RING Output

- Edge file (TSV)
- Node file (TSV)
- Network file (JSON, nodes + edges)

NodeId1	Interaction	NodeId2	Distance	Angle	Energy	Atom1	Atom2	Donor	Positive	Cation	Orientation	Model
A:7:_ILE	VDW:SC_SC	B:23:_LEU	3.863	NaN	6	CD1	CD2					1
A:10:_GLY	HBOND:MC_MC	A:14:_LEU	3.12	11.827	17	O	N	A:14:_LEU				1
A:18:_TYR	PIPISTACK:SC_SC	A:33:_PHE	5.469	163.303	9.4	-18.707,-13.286,-31.383	-15.420,-9.669,-33.838				P n2.26,p4.98	1
A:18:_TYR	PIPISTACK:SC_SC	A:37:_TYR	5.594	157.475	9.4	-18.707,-13.286,-31.383	-14.451,-11.910,-28.023				P n1.33,p4.66	1
A:18:_TYR	PIPISTACK:SC_SC	A:38:_PHE	4.872	140.138	9.4	-18.707,-13.286,-31.383	-15.755,-16.713,-29.572				T-FE n4.66,p0.97	1
A:18:_TYR	PIPISTACK:SC_SC	B:38:_PHE	6.48	42.081	9.4	-18.707,-13.286,-31.383	-18.269,-19.119,-34.170				L n4.73,p6.40	1
A:32:_ASP	IONIC:SC_SC	B:42:_ARG	3.658	41.722	20	-10.655,-13.491,-40.731	CZ		B:42:_ARG			2

Edge file for 2H9R



# PyMOL plugin (work in progress...)

- <https://github.com/BioComputingUP/ring-pymol>

