

Priyanshu Kumar

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Professional Summary

Second-year Biotechnology undergraduate specializing in computational biology and network science. Experienced in protein structure modeling, stochastic modeling, and data-driven research workflows. Currently exploring how probabilistic models and small-world networks underpin biological organization and neural computation. Passionate about building scalable, reproducible computational frameworks for structural and systems biology.

Research & Publications

bioRxiv | Submitted to *The Journal of Supercomputing* (Springer)

First Author Publication

2025

Title: "AF2Rank Revisited: Reproducing AlphaFold-Based Structure Evaluation and a Hypothesis for Context-Aware Refinement (CAR-AF)"

Status: Preprint published (DOI: 10.1101/2025.04.30.651434), under review at Springer.

- Independently reproduced and extended the AF2Rank methodology for AlphaFold-based protein evaluation, processing over 145 000 Rosetta decoy structures and deriving quantitative confidence metrics.
- Implemented local inference using JAX and TensorFlow, developing automated pipelines for reproducibility and performance scaling on limited hardware (12 GB RAM).
- Designed a reverse-classification model using XGBoost, achieving 61.5 % accuracy across 133 protein targets — validating that AlphaFold confidence metrics encode protein-specific patterns.
- Proposed the Context-Aware Refinement (CAR-AF) framework introducing environmental context into refinement loops; integrated SHAP interpretability and dimensionality reduction analysis.
- Conceptually linked model performance patterns with small-world connectivity and Markov stochastic transitions, illustrating parallels between protein networks and neural systems.

Technical Projects

AF2Rank Reproduction & Extension: • Developed a complete computational pipeline integrating AlphaFold2 outputs, Rosetta metrics, and machine-learning models in Python.

- Engineered robust data-handling workflows with NumPy/Pandas and automated evaluation notebooks for reproducibility.
- Explored stochastic modeling of protein confidence metrics and their relation to network properties and error propagation.
- Applied visualization and statistical analysis to identify small-world-like correlations between structural subspaces.

Education

Chandigarh University

Bachelor of Engineering in Biotechnology

CGPA: 8.13 / 10 (First Year)

Relevant Coursework: Computational Biology, Molecular Genetics, Bioinformatics, Systems Biology.

Punjab, India

Aug 2024 – Jul 2028

Technical Skills

Programming & Scientific Computing: Python, C++, Bash, LaTeX, Jupyter, Google Colab

Machine Learning & Modeling: TensorFlow, PyTorch, XGBoost, scikit-learn, SHAP, Optuna, stochastic simulation, probabilistic inference

Computational Biology: AlphaFold2, ColabFold, Rosetta Suite, Biopython, structural alignment, molecular visualization (PyMOL, ChimeraX)

Data Analysis & Visualization: Pandas, NumPy, Matplotlib, Seaborn, PCA/t-SNE/UMAP, statistical modeling, correlation networks

Development & Reproducibility Tools: Git/GitHub, Ubuntu WSL, VS Code, Docker, High-Performance Computing, command-line interfaces (Claude, Gemini, ChatGPT), shell scripting, automation pipelines

Collaborative & Outreach Experience

- Conducted peer sessions on genomics, small-world networks, and Markov processes using intuitive analogies to simplify complex systems.
- Led collaborative wet-lab replication experiments to improve data reproducibility and collective understanding within the Biotechnology department.
- Guided peers in using computational notebooks and open-source datasets for structural biology practice.

Achievements & Certifications

- **Tech Invent 2024:** Second Place – Developed IoT-based water-quality detection system utilizing biosensor technologies.
- **Professional Development:** Mathematics for Machine Learning (Coursera) – In Progress; Deep Learning Specialization – Ongoing.

Research Vision

Developing integrative computational frameworks that merge deep learning, network theory, and physics-based modeling to decode molecular and neural systems. Building on prior work in AlphaFold model evaluation and small-world network behavior, I aim to extend these system-level insights toward computational neuroscience and biologically inspired AI research.