

# Tools

Name	License
Mosaic	MIT
RosettaCommons Foundry (RFDiffusion + ProteinMPNN + RosettaFold3)	BSD-3
BindCraft	MIT
BoltzGen	MIT
BoltzDesign 1	MIT
Protpardelle-1c	MIT
Chroma	Apache-2.0
ODesign	Apache-2.0
PXDesign	Apache-2.0
Germinal	Apache-2.0
Protein-Hunter	MIT
ColabDesign	THE BEER-WARE 🍺

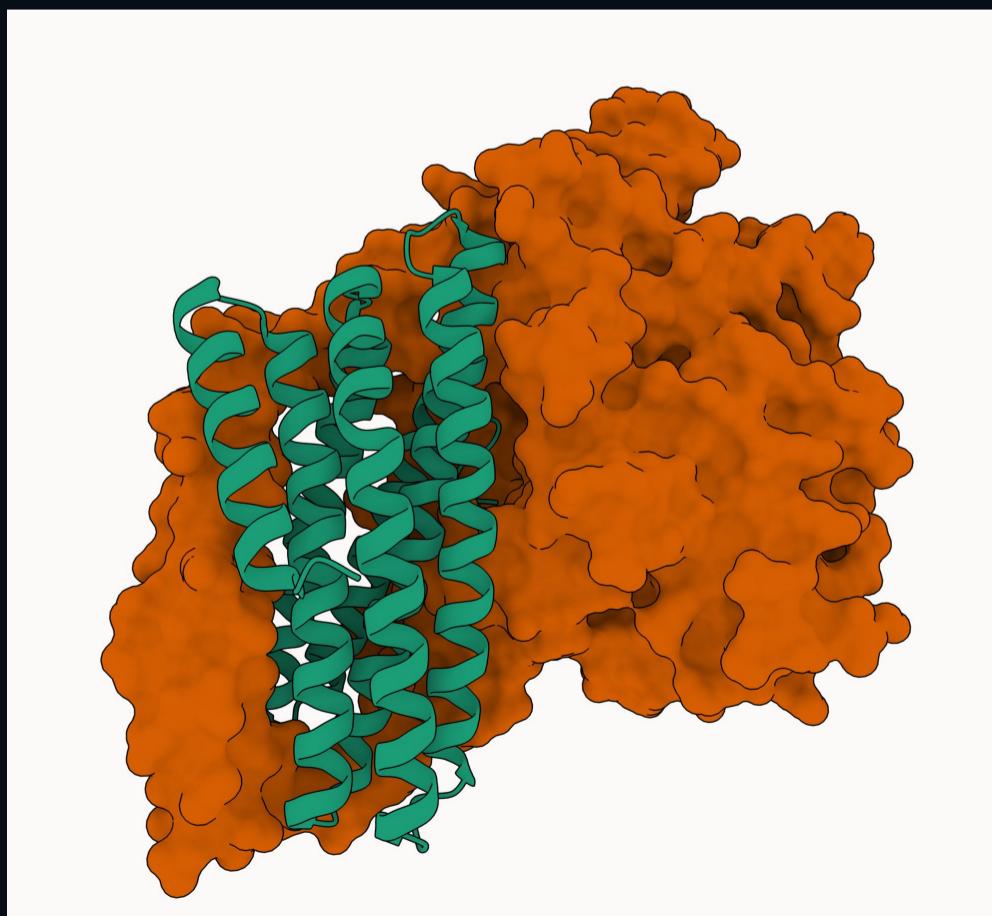
# Workflows

Name	License
Nvidia BioNeMo	Apache-2.0
ProteinDJ	MIT
BinderFlow	GPL-3.0
Ovo	MIT
ProtFlow	MIT
Nf-proteindesign	MIT

# Mosaic

Mosaic provides a modular framework for multi-objective protein design, unifying multiple machine learning models within a single, gradient-based optimization workflow.

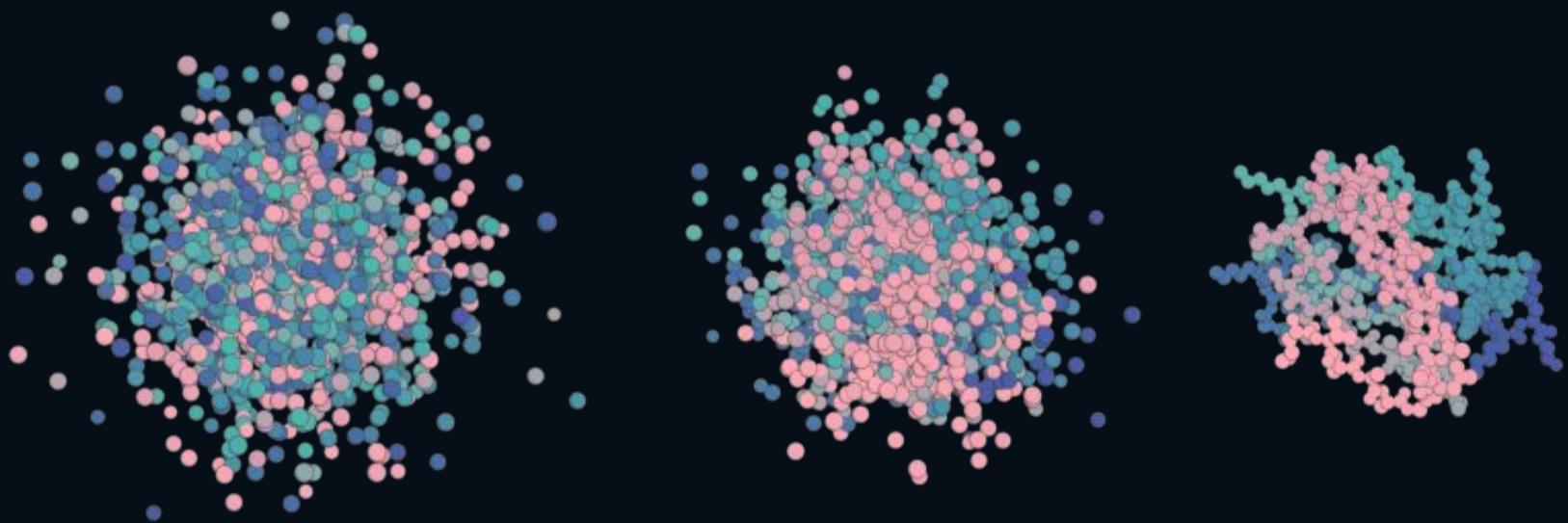
It enables simultaneous optimization of diverse protein properties-such as binding affinity, solubility, and structural stability-addressing key challenges in modern protein engineering. The framework supports integration with advanced models including AlphaFold2, Boltz, and ProteinMPNN, and allows users to define custom, task-specific loss functions to tailor design objectives to specific biological applications.



# RosettaCommons Foundry

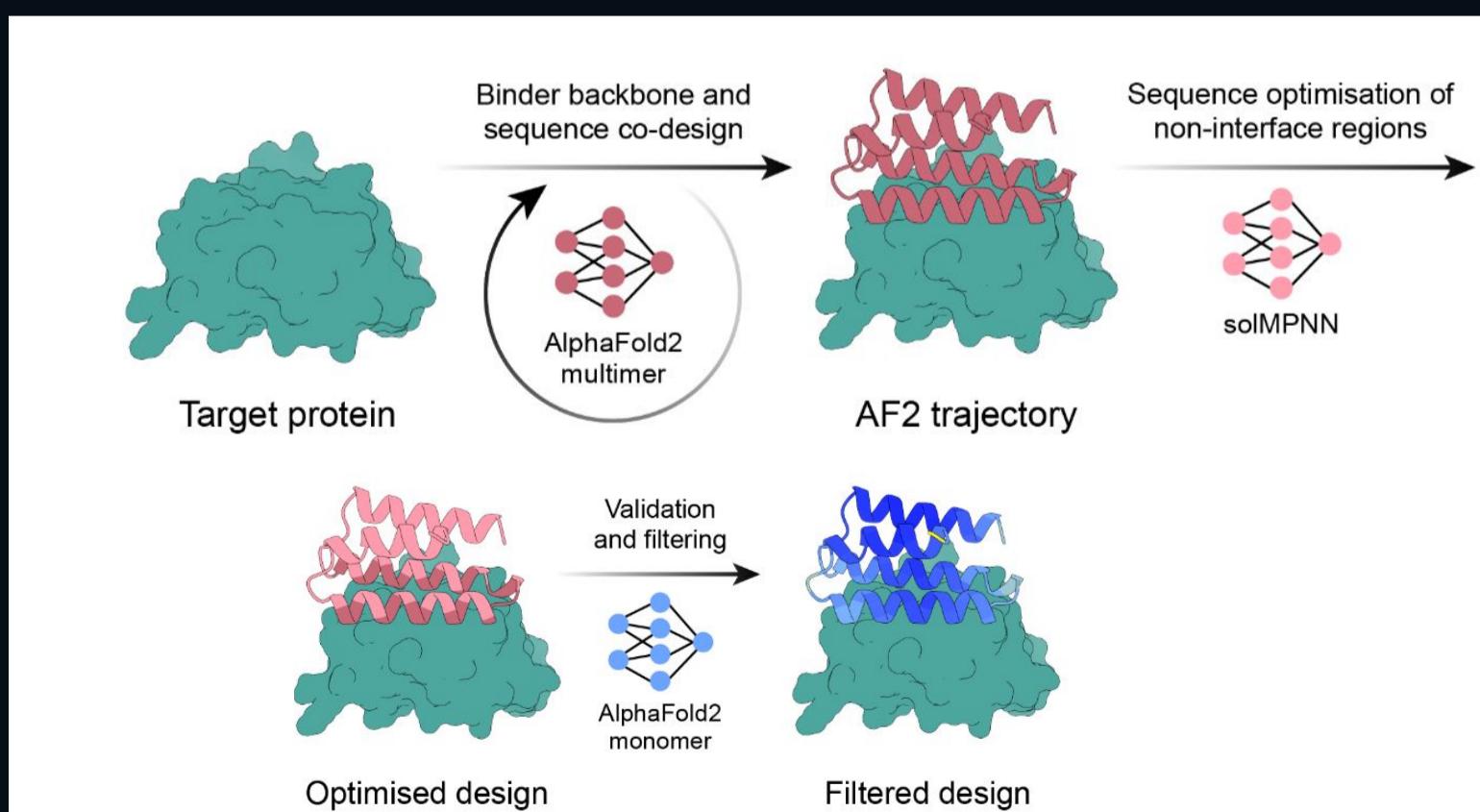
RosettaCommons Foundry is an open-source, unified biomolecular foundation model platform developed under the RosettaCommons community (& BakerLab), providing tooling and infrastructure to use and train a suite of state-of-the-art models for protein design and structure prediction.

It integrates multiple model classes-including RFdiffusion3 (all-atom generative design), RosettaFold3 (structure prediction), and ProteinMPNN/LigandMPNN (sequence design)



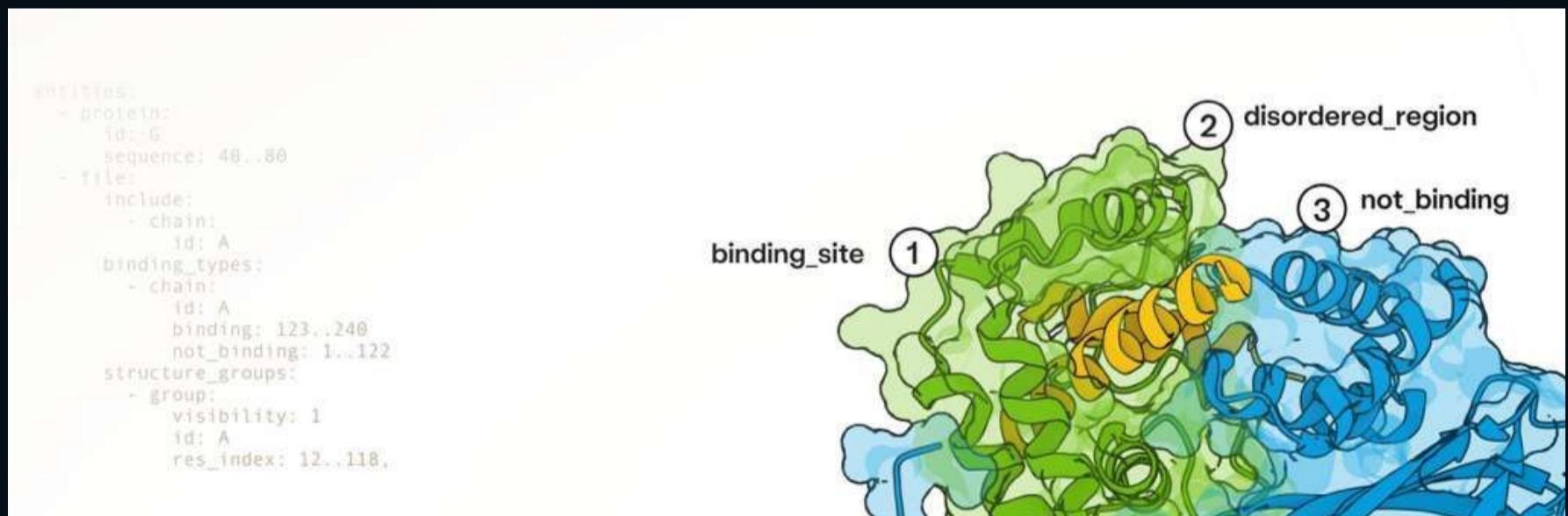
# BindCraft

BindCraft is an automated, structure-based pipeline for de novo protein binder design that aims to generate high-affinity, target-specific binders with minimal experimental screening. The workflow integrates deep learning-based backbone generation and sequence design with co-folding and confidence filtering using structure prediction models (e.g., AlphaFold-Multimer) to directly evaluate binder–target interactions in silico. By optimizing designs against structural confidence and interface metrics, BindCraft can achieve unusually high experimental hit rates, in some cases approaching one-shot success.



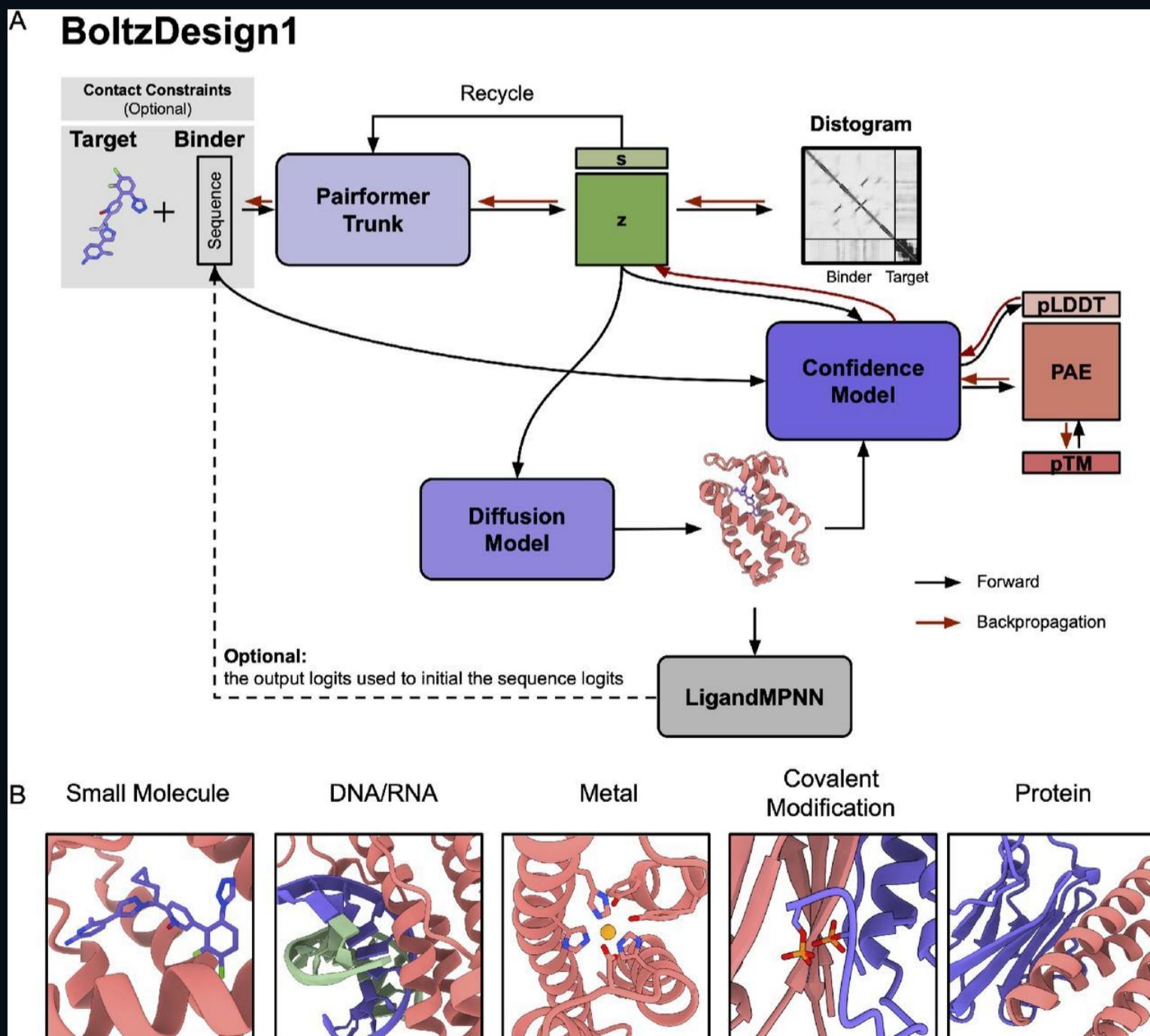
# BoltzGen

A generative AI model developed by MIT and collaborators for designing protein and peptide binders across diverse biological targets, including proteins and small molecules, by combining all-atom generative modeling with a flexible design specification language that enables controllable generation across molecular types. BoltzGen unifies structure prediction and binder design, aiming for nanomolar affinity outcomes with broad applicability



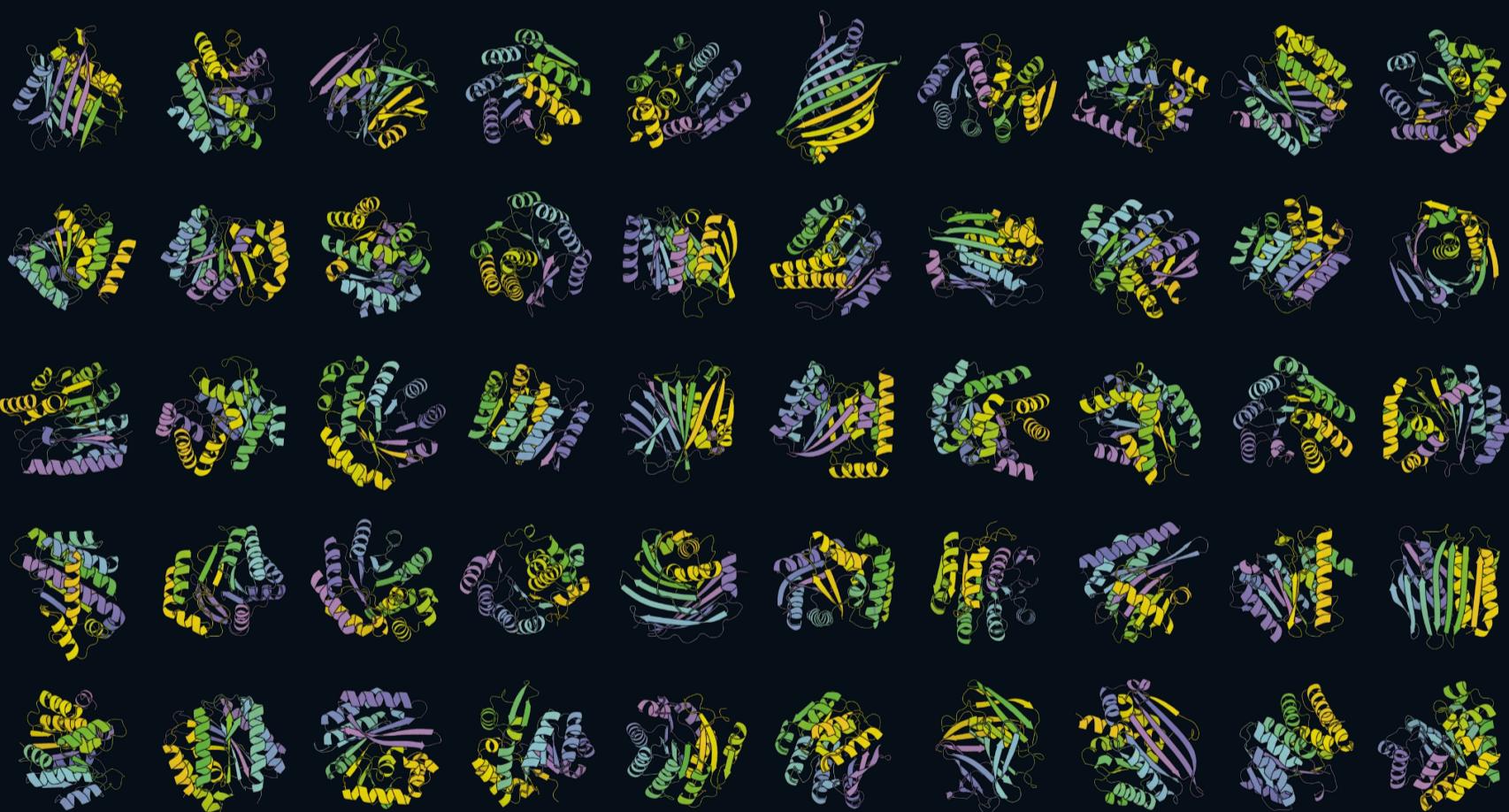
# BoltzDesign 1

A computational method that inverts an all-atom structure prediction model (Boltz) to enable binder design for broad classes of targets without model fine-tuning, optimizing distance distributions directly to bias designs toward stable, low-energy complexes suitable for biosensor, enzyme engineering, and therapeutic applications.



# Protpardelle-1c

Protpardelle-1c is an all-atom diffusion-based protein generative model that jointly designs protein structure and sequence, explicitly modeling sidechains for chemically realistic outputs. The Protpardelle-1c extension adds conditional generation, supporting robust motif scaffolding and multichain complex design, which are critical for functional protein engineering.



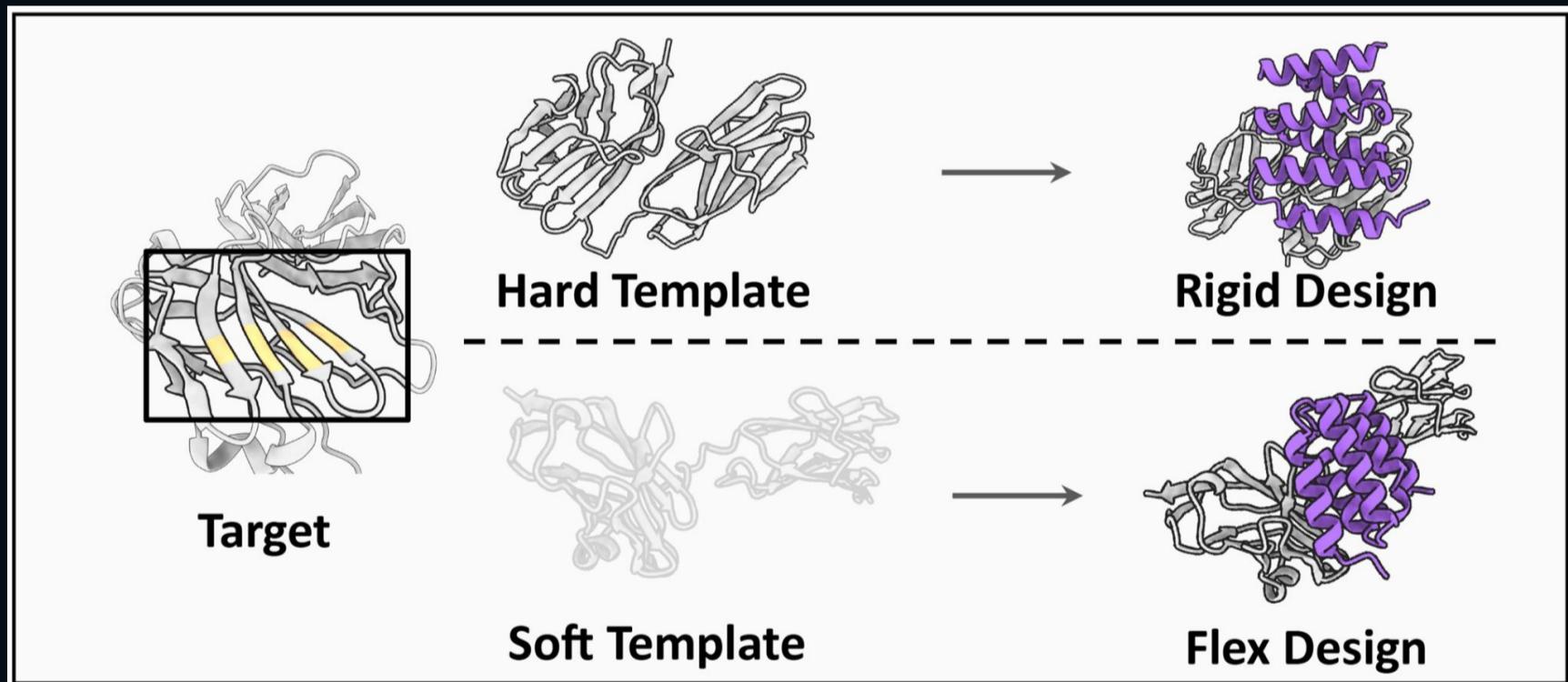
# Chroma

A generative protein design framework that uses diffusion models, graph neural networks, and programmable constraint conditioners to sample and design all-atom protein structures and sequences efficiently; it supports composable constraints for structural features like symmetry, substructures, and sequence masks.



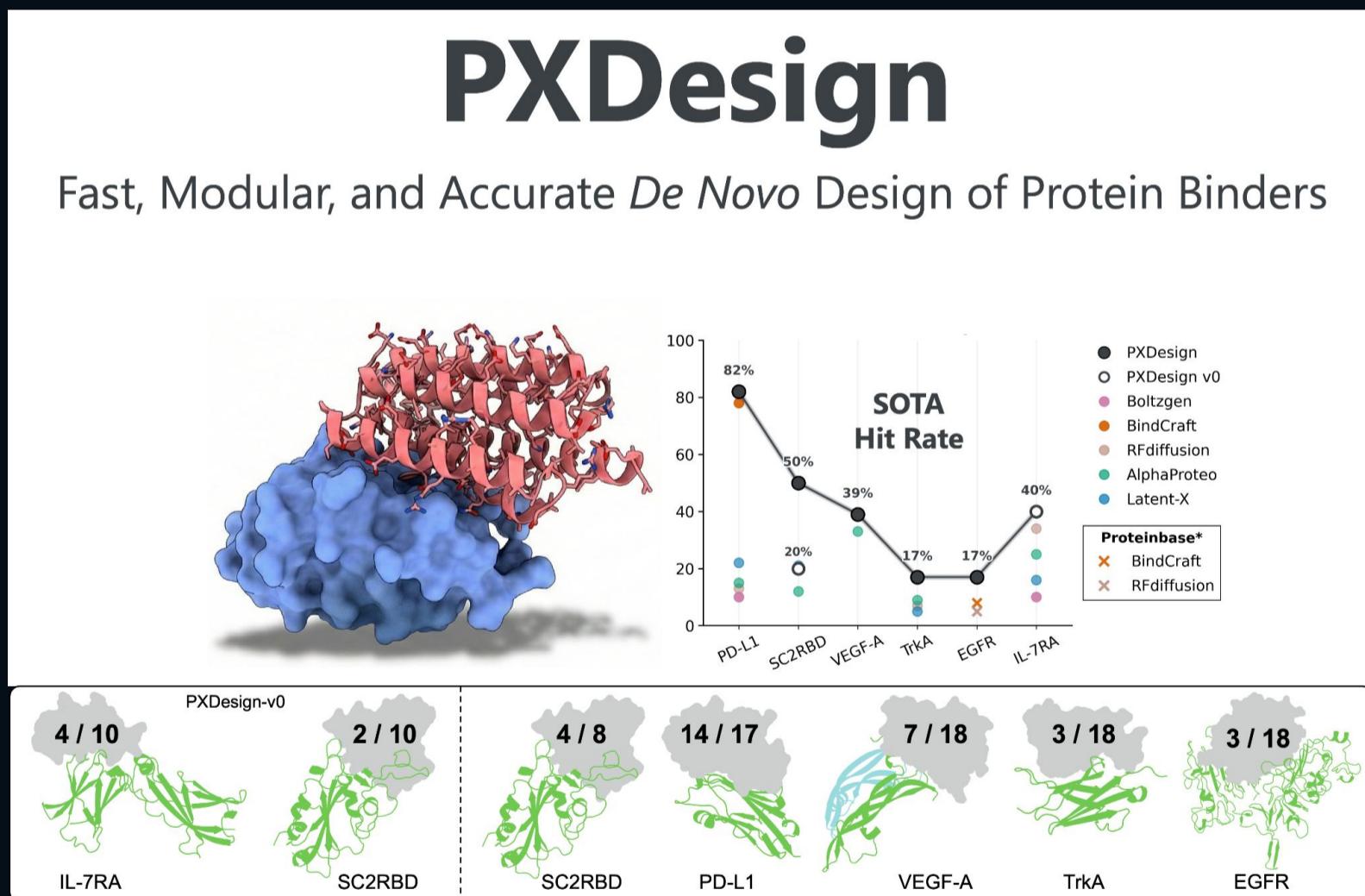
# ODesign

ODesign is a generative AI framework for multimodal, all-atom biomolecular design, capable of producing proteins, nucleic acids, and small molecules within a single model. It employs a two-stage process: a conditional diffusion module generates 3D backbones, followed by a multimodal inverse folding module that assigns sequences and atom types.



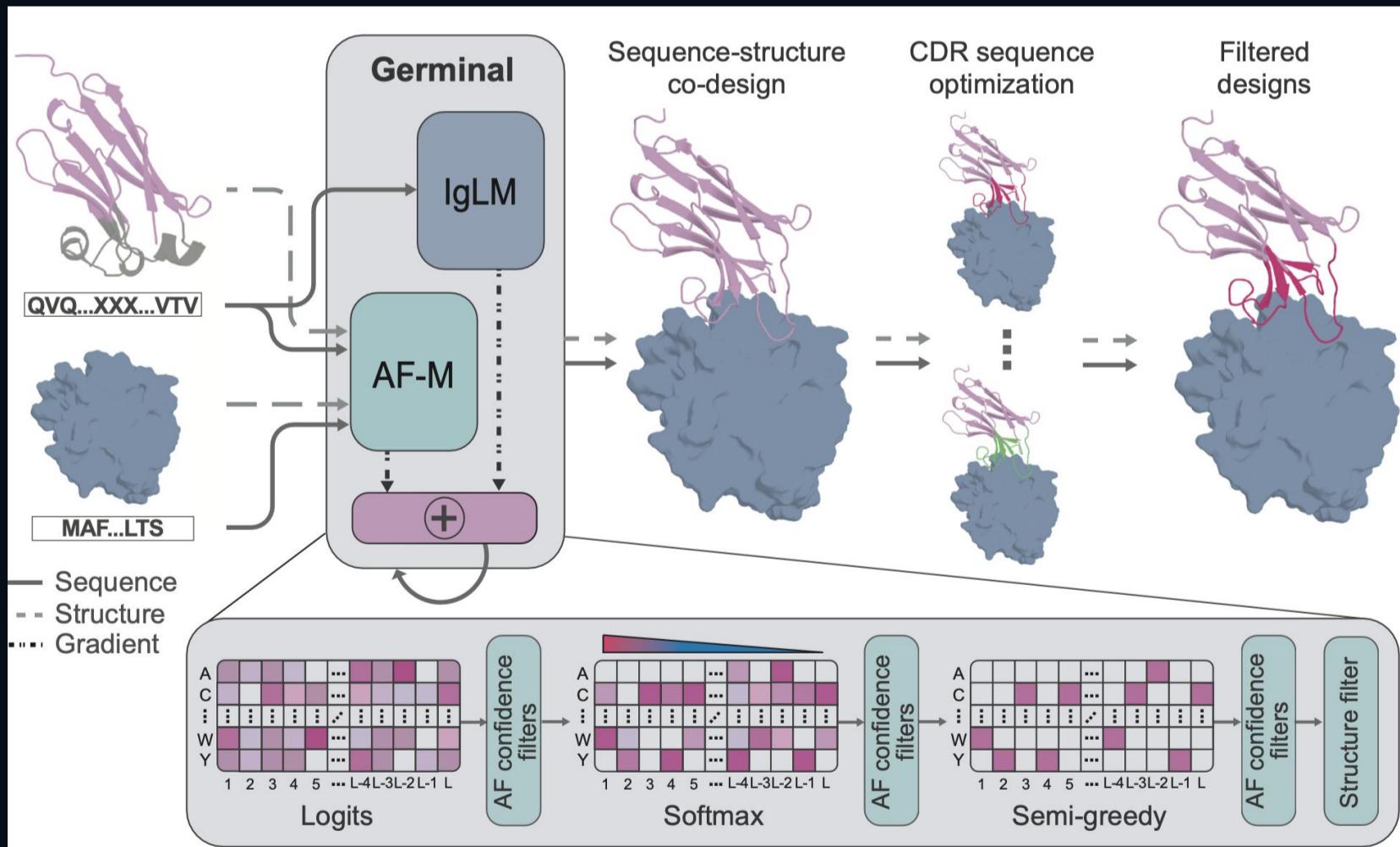
# PXDesign

A de novo protein binder design suite combining a diffusion generator (PXDesign-d) with confidence models (Protenix, AF2-IG) for generation, prediction, and filtering, achieving high nanomolar hit rates (e.g., 17–82%) on multiple diverse targets and facilitating structure-guided binder selection for experimental workflows.



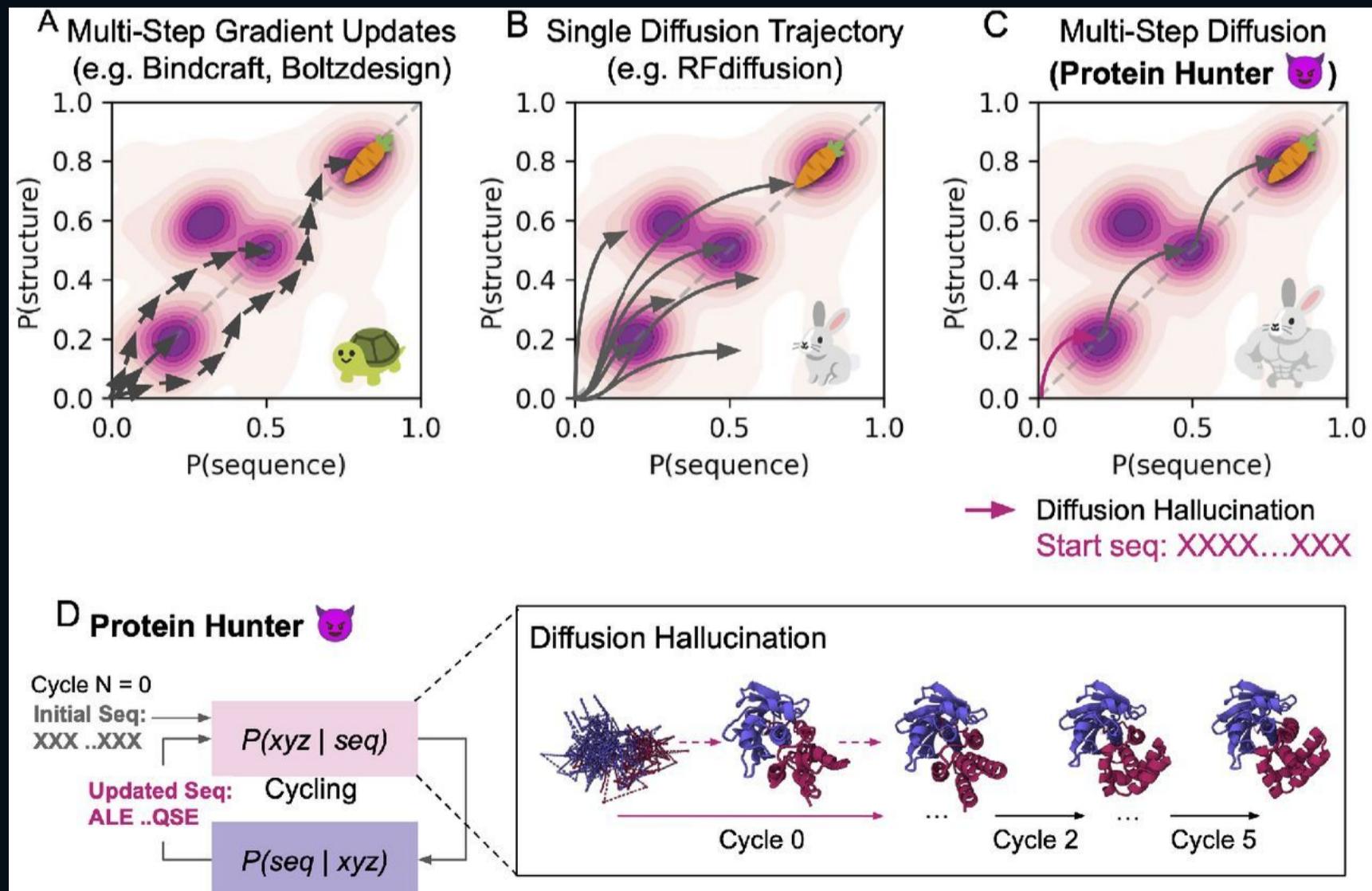
# Germinal

Germinal is an open-source generative design pipeline for epitope-targeted de novo antibody generation. The framework implements a three-stage computational workflow to produce antibody sequences and structures against defined residues (epitopes) on a target protein: (1) hallucination of initial binder structures using ColabDesign-based methods, (2) sequence redesign with a deep learning inverse-folding model (AbMPNN), and (3) co-folding and structural evaluation with a high-accuracy structure prediction model.



# Protein-Hunter

Protein Hunter is a novel computational framework designed for efficient de novo protein design by repurposing the "hallucination" capabilities of diffusion-based structure prediction models. Instead of relying on slow, gradient-based optimization, this method initiates the design process using a sequence of unknown "X" tokens to generate high-quality backbone structures. The system employs an iterative cycling strategy that alternates between structure prediction and sequence redesign using ProteinMPNN, progressively refining the compatibility between the two.



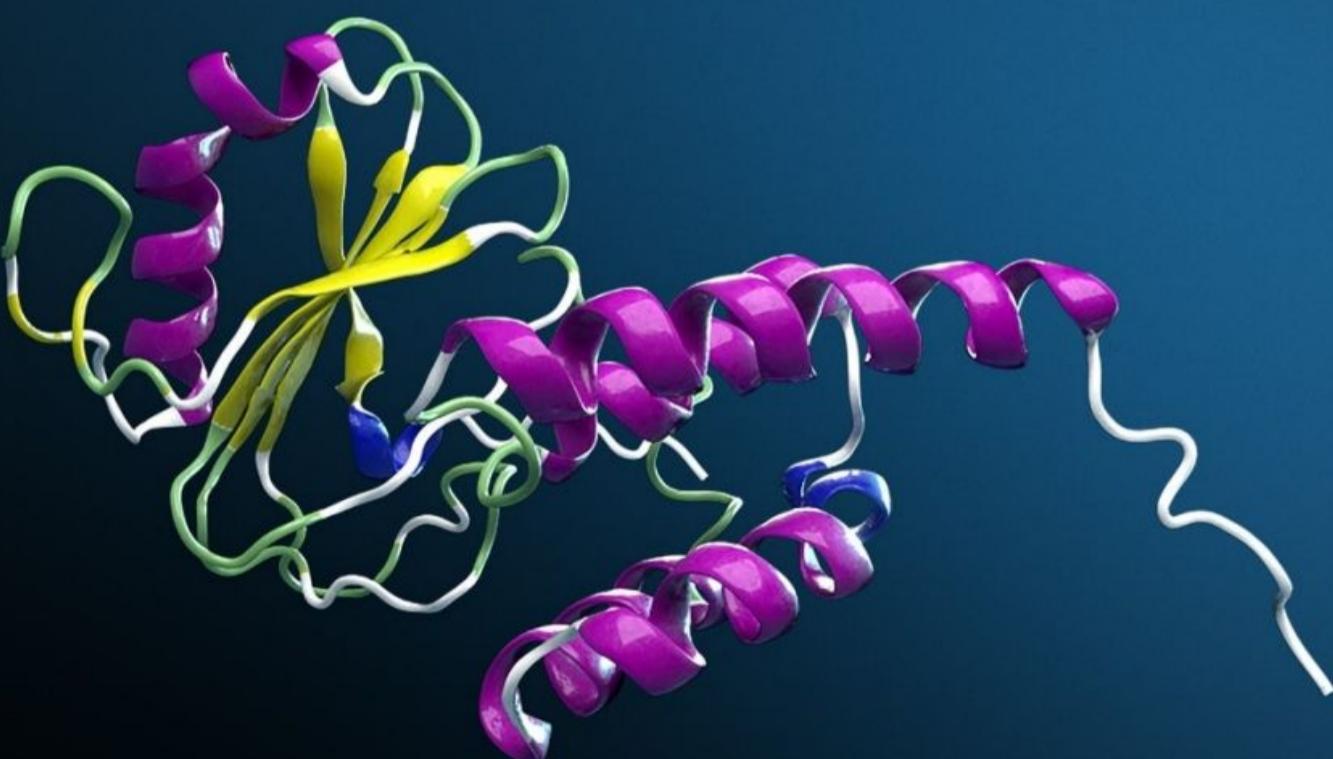
# ColabDesign

ColabDesign is an open-source computational protein design framework that makes deep learning-based design methods accessible via Jupyter/Google Colab interfaces. It integrates multiple generative and predictive models to support different aspects of protein design by operating across key probability spaces, such as structure conditioning on sequence, sequence conditioning on structure, and de novo structure generation.



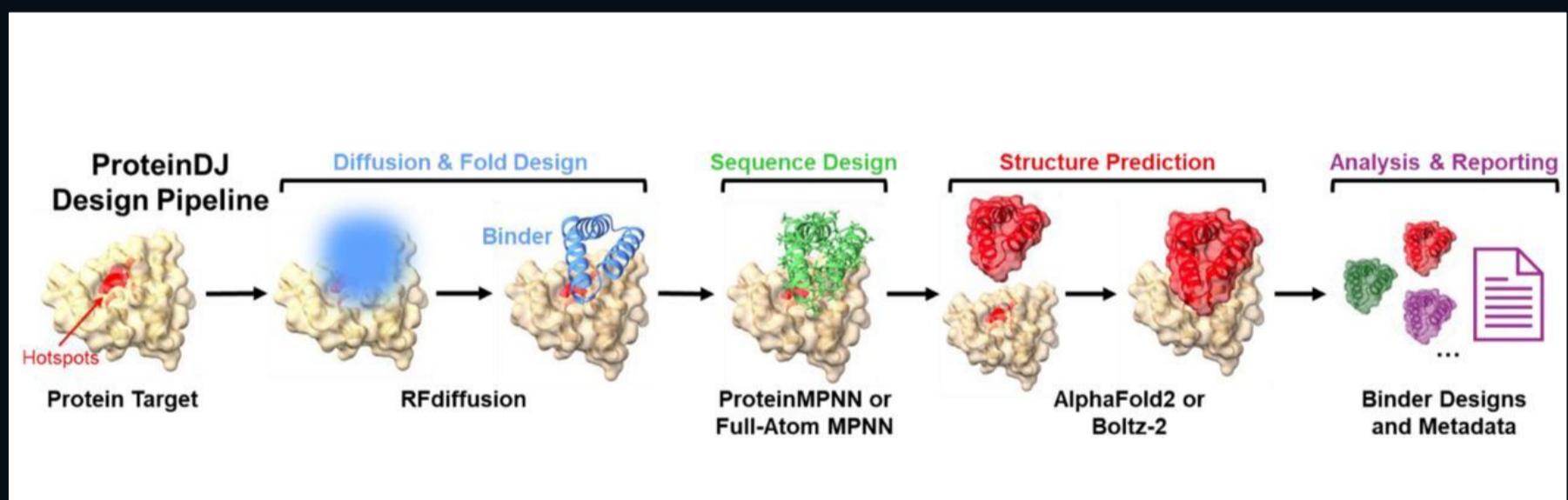
# Nvidia BioNeMo

NVIDIA BioNeMo supports protein binder design by providing a GPU-accelerated environment for generative modeling, structure prediction, and sequence optimization. It integrates state-of-the-art models (e.g., diffusion-based backbone generation, inverse folding with ProteinMPNN-like methods, and AlphaFold-class structure evaluation) into scalable workflows for designing and screening protein-protein interactions. Running on multi-GPU infrastructure, BioNeMo enables high-throughput generation, refinement, and validation of candidate binders, significantly accelerating the design-evaluate cycle compared with traditional pipelines.



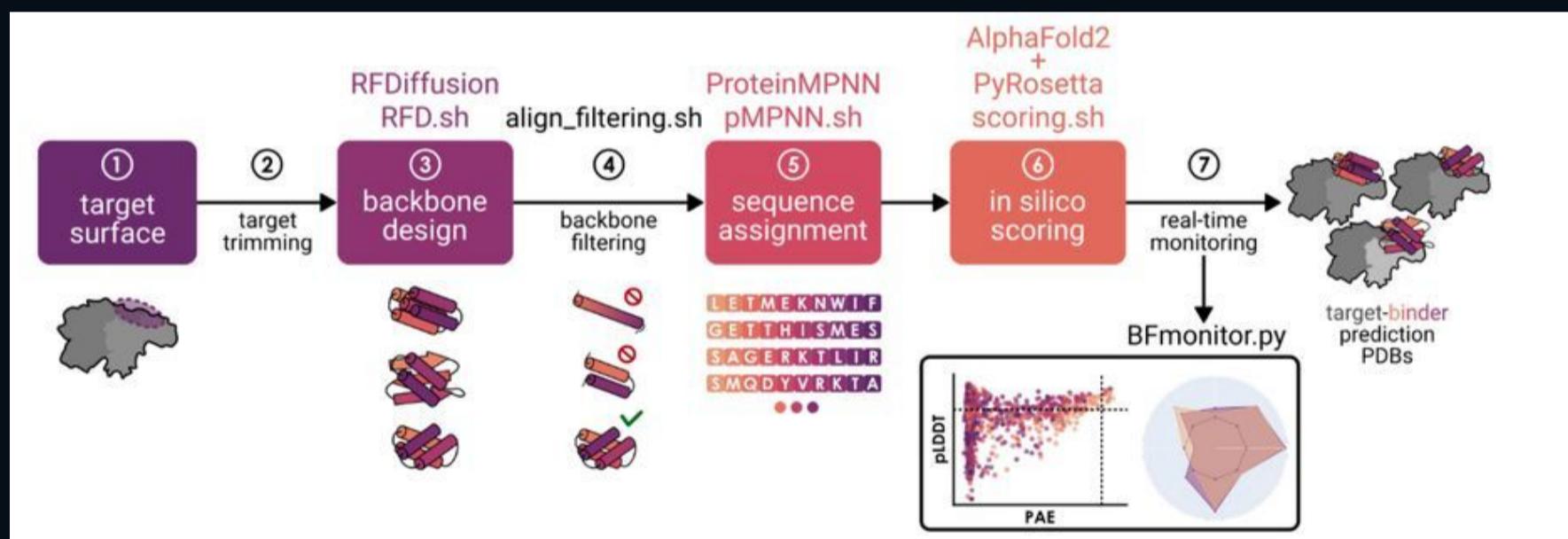
# ProteinDJ

A high-performance, modular protein design pipeline implemented with Nextflow for scalable execution on HPC systems, integrating deep learning models (e.g., RFdiffusion for backbone generation, ProteinMPNN or Full-Atom MPNN for sequence design, and structure prediction tools like AlphaFold2/Boltz) to automate de novo binder design campaigns with parallel workload distribution.



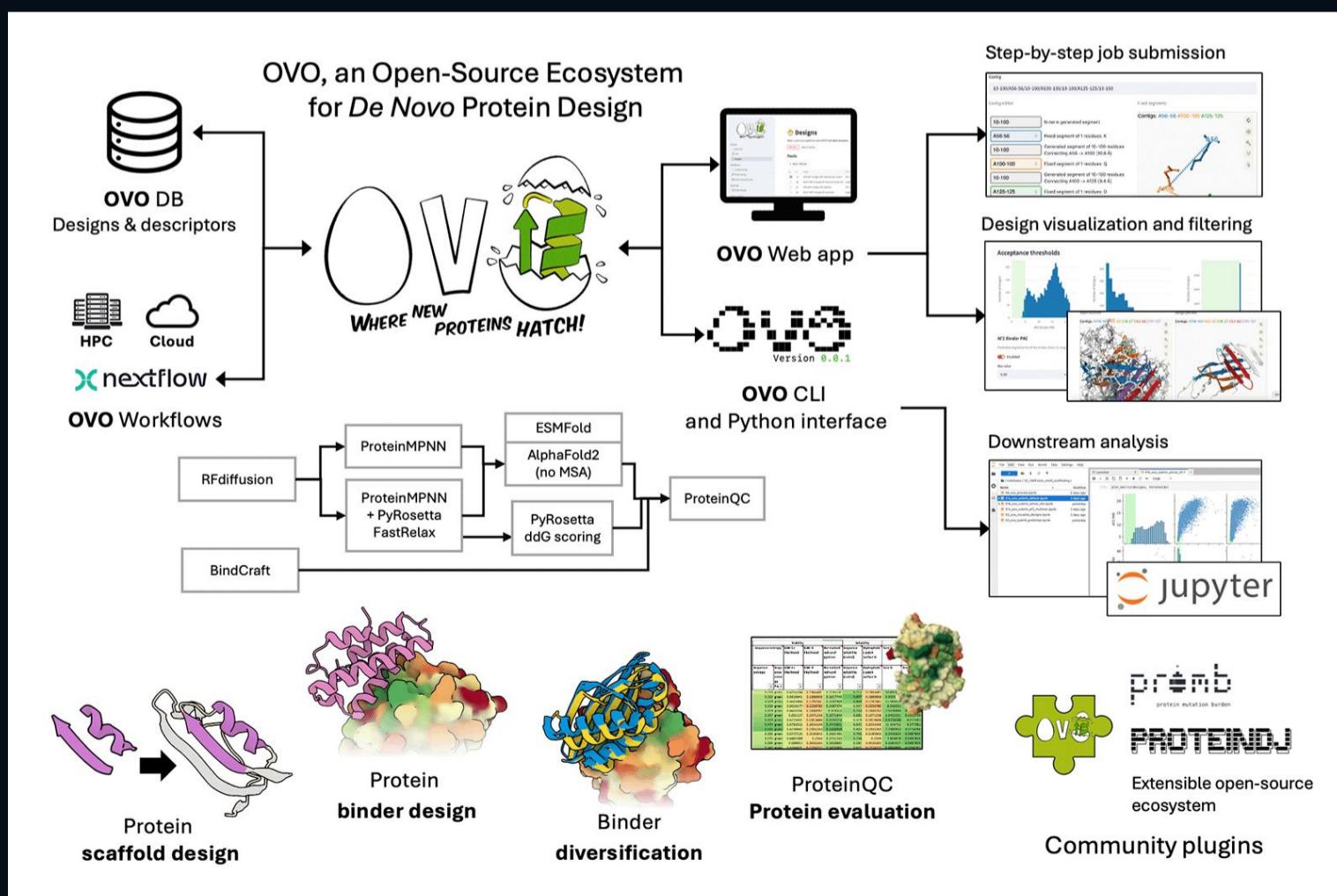
# BinderFlow

An automated, modular workflow for end-to-end protein binder design that structures and parallelizes all design steps (backbone generation, sequence assignment, scoring, and monitoring) into batch jobs, enabling efficient GPU utilization, real-time campaign tracking, and scalable candidate generation for experimental validation.



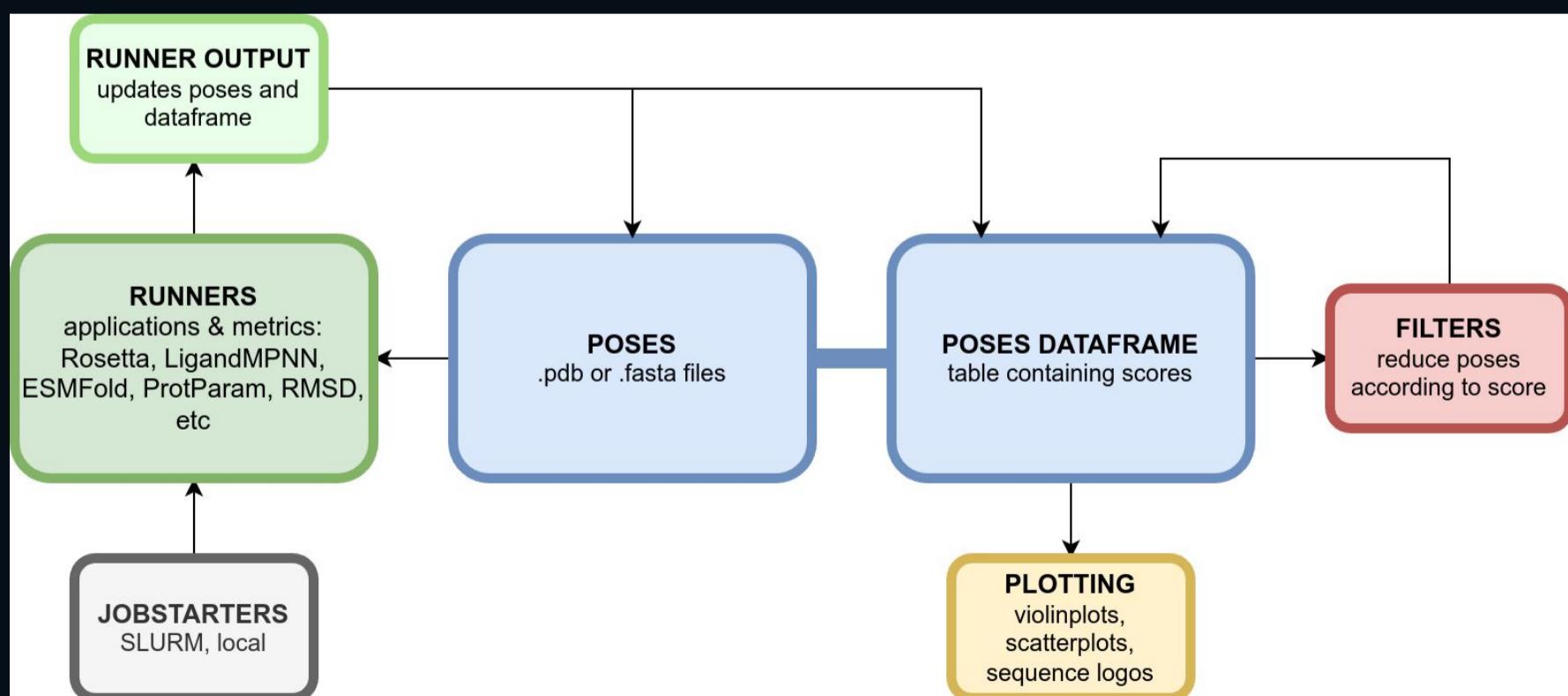
# Ovo

An open-source ecosystem for de novo protein design that consolidates a variety of models, workflows, data management, and visualization tools into a scalable, infrastructure-agnostic platform, enabling users to orchestrate scaffold design, binder design, diversification, and validation via both command-line and graphical interfaces. Ovo integrates quality control modules to evaluate sequences and structures, supports seamless incorporation of community-developed plugins, and provides interactive visualization to manage and benchmark large sets of designs.



# ProtFlow

ProtFlow is an open-source Python framework for protein design that provides modular workflow construction, unified protein objects, and standardized tool wrappers. It supports execution on local machines, HPC clusters, or cloud environments. The framework includes a flow-matching generative model that produces protein sequences from latent embeddings, enabling efficient design of peptides, single-chain proteins, and multichain complexes such as antibodies. ProtFlow standardizes scoring, metadata tracking, and pipeline execution to improve reproducibility and scalability in protein design projects.



# nf-proteindesign

nf-proteindesign is an open-source Nextflow pipeline developed by Seqera Labs for automated protein design tasks. It uses Boltzgen to generate novel protein binders, nanobodies, and peptides for given target structures, and it can optionally run ProteinMPNN to optimize sequences, Boltz-2 for structural refolding, IPSAE for interface quality scoring, PRODIGY for binding affinity prediction, and Foldseek to search structural databases for similar designs.

