■ Docking Pipeline Installation & Setup Guide

1■■ Install Python 3

Check version:
python3 --version
If older than 3.9:
sudo apt update
sudo apt install -y python3 python3-pip python3-venv

2■■ Install Miniconda

cd ~/Downloads
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
bash Miniconda3-latest-Linux-x86_64.sh
Then restart shell or run: source ~/.bashrc

3■■ Create and Activate Conda Environment

conda create -n docking_env python=3.12 -y
conda activate docking_env

4■■ Install Open Babel

conda install -c conda-forge openbabel -y
Confirm: obabel -V

5■■ Install AutoDock Vina

conda install -c conda-forge autodock-vina -y
Confirm: vina --version

6■■ Enable Bioconda (Optional)

conda config --add channels defaults
conda config --add channels bioconda
conda config --add channels conda-forge

7■■ Install RDKit (Optional)

conda install -c conda-forge rdkit -y

8■■ Install UCSF ChimeraX (Optional)

Download from: https://www.cgl.ucsf.edu/chimerax/download.html
Or:
wget https://www.cgl.ucsf.edu/chimerax/downloads/ChimeraX-1.8-linux_x86_64.bin
bash ChimeraX-1.8-linux_x86_64.bin
Launch: chimerax

9■■ Verify Installation

python3 --version
conda list | grep vina
obabel -V
vina --version

■ Export Environment (Optional)

Create shareable YAML:
conda env export --name docking_env > environment.yml
Recreate later:
conda env create -f environment.yml

■ You are now ready to run the docking pipeline!

Proceed with editing your docking_config.yml and running:
python3 run_pipeline.py docking_config.yml