

Vina command sheet

A worked configuration file and the driver pattern. Keep the configuration file with the output.

Configuration file

Line	Meaning
receptor = receptor.pdbqt	The prepared receptor
ligand = ligand.pdbqt	The prepared ligand
center_x, center_y, center_z	Box centre, often the centroid of the crystal ligand
size_x, size_y, size_z	Box size in Angstroms, large enough for the ligand to rotate
exhaustiveness = 24	Search effort, raise it for flexible ligands
num_modes = 20	How many distinct poses to report
seed = 42	Recorded so that the run repeats
out = poses.pdbqt	Where the poses are written

Driving it from a notebook

- Run the program with subprocess, passing the configuration file, and capture the standard output into a log file
- Or use the Python bindings, setting receptor, ligand and box, then compute and dock
- Read the pose file back for viewing and for deviation measurement
- Record the top score, the spread of the top three, and whether the poses cluster in one site

Reading the output

Column	What it tells you
Mode	Rank of the pose
Affinity in kilocalories per mole	The docking score, a prediction and not a measurement
Deviation lower and upper bound	How far each pose sits from the best one
Spread of the top three	Whether the search settled on one site or could not distinguish several

Based on the ERAS Africa Molecular Docking using Python course, 2026, and the study "Target Protein Pocket Volume and Antiretroviral Drug Physicochemical Properties" (Hailekiros, 2026) with its reproduction guide. Tool documentation from RDKit, AutoDock Vina, Meeko, RCSB PDB, PubChem and ProteinsPlus. Free to copy and adapt with attribution.