

Grid pocket volume method card

Four steps, the copy rule, and the two validations that make a simple method publishable.

The method

Step	What happens	Why
1 Grid	Points spaced half an Angstrom are laid around the bound ligand	A fine grid measures small cavities
2 Distance filter	Only points within five Angstroms of ligand atoms are kept	Restricts the region to that pocket
3 Atom exclusion	Points inside the van der Waals radius of a protein atom are removed	That space is occupied and cannot hold ligand atoms
4 Count	Surviving points times the volume of one cube	Gives the pocket volume in cubic Angstroms

The copy rule

- Count the copies of the ligand in the structure and print the count in the output.
- Measure the pocket at every copy and report the average across copies.
- Summing across copies describes the assembly rather than one pocket and inflates the value.
- In this project an earlier version summed rather than averaged, which inflated two of five results. The error was found, corrected and disclosed.

The two validations

Validation	What was done	What it shows
Redocking	The known ligand was removed and docked again from scratch	The measured region is where the drug really binds
Independent tool	The same structures were measured by a published tool from another group	Agreement in ordering across independently built methods

Reference values

Target	Entry	Ligand	Grid volume	Independent tool
Reverse transcriptase	3MEE	Rilpivirine	1331	517
Integrase	8W09	Integrase inhibitor	1702	872
Envelope gp120	8CZZ	Temsavir	1726	892
Protease	4YOA	Darunavir	2916	594
Capsid	7RHN	Lenacapavir	3459	1048

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.