

Docking run checklist

One page per run. A run without this page is not reproducible.

Target and structure identifier		Ligand	
Run name		Date	

Preparation

Item	Done	Note
Chains kept and chains removed recorded		
Waters and additives removed, or a retained water justified		
Hydrogens added at physiological pH		
Ligand protonation state set and checked		
Stereochemistry of the prepared ligand checked visually		
Prepared files saved with the run		

Parameters

Box centre		Box size	
Exhaustiveness		Number of modes	
Random seed		Program and version	

Validation

Check	Result
Redocking of the known ligand performed	
Root mean square deviation from the crystal pose	
Criterion set in advance and met	
Stability across three seeds	
Warnings in the log reviewed	

- Validation comes before prediction. A protocol that cannot reproduce a known pose cannot support a prediction in that system.

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.