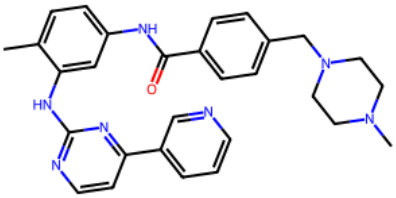
Astinova AI Platform — Molecular Docking Report

Ligand: imatinib (public) · Target: ABL1 kinase (PDB 2HYY, public) · pose prediction & binding analysis

Illustrative sample on a public target/compound — for format demonstration.



Property	Value
Target	ABL1 tyrosine kinase (PDB 2HYY)
Grid	centred on ATP site, 22 A box
Ligand MW	493.6 Da
Rotatable bonds	7
Poses scored	20

Top docking poses

Pose	Score (kcal/mol)	Key interactions	RMSD to top (A)
1 (best)	-11.4	H-bond Met318 hinge; Thr315 gatekeeper; DFG-out hydrophobic	0.00
2	-11.1	Hinge H-bond retained; slight solvent-front shift	0.9
3	-10.6	Hinge H-bond; piperazine flips to solvent	1.6
4	-10.2	Alternate hinge donor; weaker gatekeeper contact	2.4

The top-ranked pose reproduces the canonical Type-II binding mode: a hinge hydrogen bond to Met318, contact with the Thr315 gatekeeper, and occupancy of the DFG-out allosteric pocket. Scores and interactions are docking estimates and should be confirmed by rescoring / MD and, where possible, an experimental assay.