

Astinova AI Platform — Structure Prediction Report

Complex: EGFR kinase domain + gefitinib (public) · co-folding & confidence assessment

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

Prediction confidence

Metric	Value	Interpretation
pTM	0.88	High overall fold confidence
ipTM (interface)	0.71	Reliable ligand-interface placement
Mean pLDDT (pocket)	86	Well-resolved binding site
PAE (interface, A)	3.9	Low interface positional error
Ranking model	1 of 5	Top-ranked of 5 sampled models

Co-folding places the ligand in the ATP cleft with a hinge contact consistent with the known binding mode; high pTM/ipTM and low interface PAE indicate a confident prediction. Predicted structures should be validated against experimental data (X-ray / cryo-EM) before use in design.