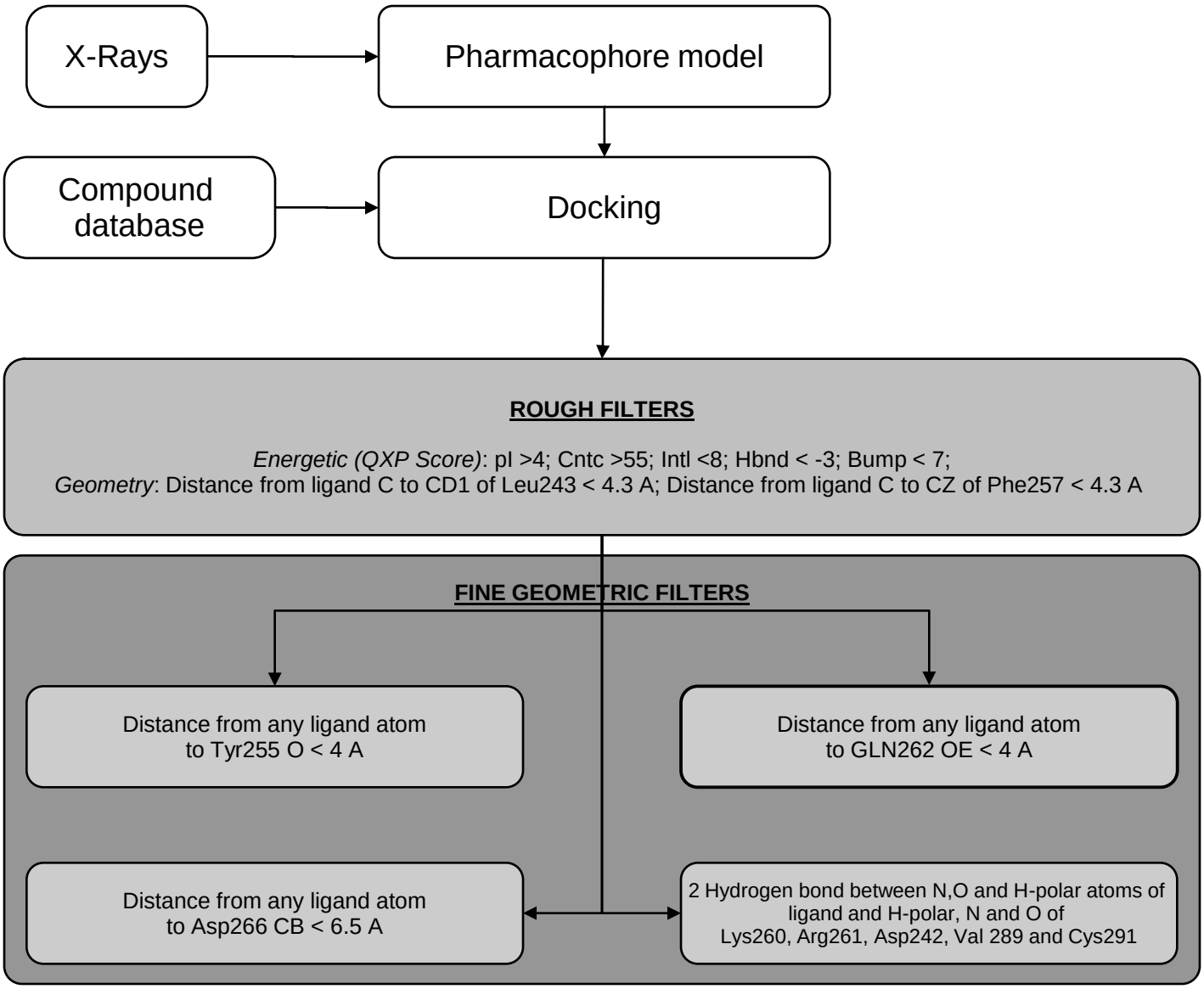
X-Rays
Pharmacophore model
Compound database
Docking
ROUGH FILTERS
Energetic (QXP Score): pI >4; Cntc >55; Intl <8; Hbnd < -3; Bump < 7;
Geometry: Distance from ligand C to CD1 of Leu243 < 4.3 A; Distance from ligand C to CZ of Phe257 < 4.3 A
FINE GEOMETRIC FILTERS
Distance from any ligand atom to Tyr255 O < 4 A
Distance from any ligand atom to GLN262 OE < 4 A
Distance from any ligand atom to Asp266 CB < 6.5 A
2 Hydrogen bond between N,O and H-polar atoms of ligand and H-polar, N and O of Lys260, Arg261, Asp242, Val 289 and Cys291