Using DelPhi to calculate electrostatic component of solvation energy

In this example set we demonstrate how to calculate electrostatic component of solvation energy i.e. ΔG_p for a single atom and a real protein. The case of single atom (a charged sphere) is considered because there is an analytical solution via Born formula of charged ion, and the numerical solution provided by DelPhi can be compared with the analytical. In this section we also provide examples of computing electrostatic solvation energy using traditional two-dielectric model as well as the Gaussian-smooth dielectric function PBE. The corresponding files can be found in directory `Example_3.1.1/` and sub directories there in.