

Using DelPhi to compute Electrostatic component of binding energy

To demonstrate how to use DelPhi for computing electrostatic component of protein-protein binding we have taken barnase-barstar as the system. First we are required to prepare the coordinate, charge, size and parameter files for each of the three cases one for each complex (here barnase-barstar complex), receptor (protein-1 here say barnase) and ligand (protein-2 here say barstar). The required files are provided in directory `Example_3.1.6/`. This folder should have the following five files (`barnase-barstar.pdb`, `barnase.pdb`, `barstar.pdb`, `c22.crg` and `c22.siz`) and two directories (`2-dielectric/` and `gaussian/`). The `.pdb` and `.crg` files contain the coordinate information and partial charge of the all atoms respectively for the barnase-barstar, barnase and barstar systems. In the present example we will use partial atomic charges and atomic van der Waals radii from provided `c22.crg` and `c22.siz` files respectively for constituent atoms in the systems.