

## W0135

**High Resolution Protein Crystallography and Electrostatic Interaction Energy Computation.** A. Lagoutte, B. Guillot, V. Pichon-Pesme, C. Jelsch, C. Lecomte; LCM3B, UHP Nancy I, 54506 Vandoeuvre-les Nancy, France.

The PDB records show the number of (ultra-)high resolution biological macromolecules X-ray structures increasing quickly. Feasibility of multipolar refinement of such structures has been proved [Jelsch, *PNAS* 97 2000], assuming sufficiently low thermal motion. The Hansen & Coppens model gives an analytical representation of the charge density. It enables the experimental estimation of electrostatic potential and electrostatic interaction energy, which are of major importance in many biological processes. Computing electrostatic interaction energy could help to analyze structure-function relationships and protein activity.

We will present three methods to calculate protein-ligand electrostatic interaction energy. The first one uses multipolar parameters in a Buckingham's summation. The second one uses a first order interaction coulombic energy using virtual atoms. The third method, developed in our software, is a numerical integration of the product of a ligand charge density and a protein electrostatic potential, both obtained from the MoPro software [Jelsch, *JAC* in press]. We will present our results on a protein-ligand complex.

The protein electron density parameters will be either refined or transferred from our database [Pichon-Pesme; *ActaCryst* A60 2004].