

E0045

Ligand, Inhibitor–Protein Electrostatic Energy Calculations from Ultra High Resolution Refinement: MoPro Refinement Program. C. Lecomte, A. Lagoutte, B. Guillot, C. Jelsch, LCM³B, UHP Nancy 1, Faculté des Sciences, BP 239, F-54506 Vandoeuvre-lès-Nancy, claude.lecomte@lcm3b.uhp-nancy.fr.

With the increasing number of biological structures solved at high resolution, a refinement tool which allows to extract all the new information available is necessary (H positions, thermal motion, accurate stereochemistry, electron density ^[1], partial charges ^[2] and very recently interaction energies). All this information is now easily available using latest developments of the refinement program Mopro ^[3] as soon as the experimental resolution is less than 1 Å and the thermal displacement parameters not too high. The strategies for obtaining these properties will be presented. The limitations for resolutions between 1.5 and 1 Å will also be discussed in relation with our electron density data base ^[4] which is being built in Nancy.

[1] C. Jelsch, M. Teeter, M. Lamzin, V. Pichon-Pesme, R.H. Blessing & C. Lecomte, *PNAS* (2000) 97, 3171

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[3] C. Jelsch, B. Guillot, A. Lagoutte & C. Lecomte, Advances in protein and small molecule charge density refinement using Mopro, *J. Appl. Cryst.* (2005) 38, 38

[4] V. Pichon-Pesme, C. Lecomte & H. Lachezar, *J. Phys. Chem.* (1995) 99, 6242