HipHop. A Novel Refinement Method for Protein Structures

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A novel refinement method called HipHop refinement is described. Although HipHop refinement seems to be similar to simulated annealing refinement it is based on a different philosophy - namely that it is in principle impossible to determine a complete structure at a limited resolution. Thus, the limited resolution and the inaccuracy of the underlying X-ray data cause not only errors in the refined structural parameters but principal structural errors in the single model, which is usually used to explain the data.

HipHop refinement is performed in several steps. In the first step, a proper number of pseudo waters corresponding to maxima in the difference Fourier map is added to the model (HIP step, **H**$_2$O **i**n**p**ut). In the next step, the model is refined and waters not fulfilling density, shape or position criteria are removed from the model (steps HOP, **H**$_2$O **o**ut**p**ut). The process is in fact jumping between local minima – HipHop. During HipHop cycles not only the water arrangement but also side/main chain orientation is changed. The best presentation of HipHop refinement is a multi conformer PDB file.

The method was tested on several different protein structures with excellent results [1,2] The programs are available on http://www.img.cas.cz/hiphop/.

[1] Ondráček J., Weiss M.S., Mesters J.R., *Acta Cryst*., manuscript *in preparation*. [2] Ondráček J., Weiss M.S., Brynda J., Fiala J., Jursík F., Řezáčová P., Jenner L.B., Sedláček J., *Acta Crys., submitted for publication.*

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