m34.p06

Recognition of Secondary Structural Elements in low-resolution crystallographic electron density maps

Gerrit G. Langer, Olga V. Kirillova, Victor S. Lamzin

European Molecular Biology Laboratory, c/o DESY, Notkestrasse 85, 22603 Hamburg, Germany

Keywords: model building, low resolution, protein secondary structure

A crucial point in enabling automated protein model building at low resolution is to automatically obtain a good starting model together with its associated restraints for refinement. Having such a model, additional parts of the molecule can then be constructed iteratively. As a starting model the recurring motifs of helices and strands are a good choice due to their pronounced features even at low resolution. For the treatment of crystallographic electron density maps at low resolution ranging down to 4 Å the version 6.1 of the ARP/wARP software suite [1] contains a dedicated module that will trace the respective portions of the protein main thus reducing the need for manual intervention. The key elements of the method for accomplishing this task are successive filtering steps based on discriminant analysis applied to geometric features of helical fragments of increasing size. The helix building software has been applied to more than a thousand test cases from the PDB and, on average, more than 60% of the helices could be correctly identified, more than 80% of which were predicted with the correct chain direction. Furthermore the results are nearly independent of the resolution of the data. A similar approach can be used for the location of strands and results of new developments in terms of a more complete capture of secondary structure will be presented. Finally we will show, how the models built with the module can be made use of in successive steps of protein model building.

[1] Morris, R.J., Perrakis, A. & Lamzin, V.S. (2003). Methods Enzymol. 374, 229-244.

m34.p07

HAPPy - an Experimental Phasing and Model Building Pipeline from CCP4

Daniel Rolfe[a], Charles Ballard[a], Paul Emsley[b]

[a]CCP4, Computer Science and Engineering Department, CCLRC Daresbury Laboratory, UK. [b] Structural Biology Laboratory, York University, UK. E-mail: d.j.rolfe@dl.ac.uk

Keywords: software, phasing, structure solution

HAPPy (Heavy Atom Phasing in Python) is a new experimental phasing pipeline being developed by CCP4. It is a successor to Paul Emsley's CHART package. The goal is to take integrated and merged data (structure factor amplitudes), determine the heavy atom structure and phases, then take the density map through automated model building to a good (if not final) model. HAPPy will take a simple XML description of the processed data and attempt to obtain a density map suitable for model building. The first release will handle SAD data only, with further modes (e.g. MAD, MIR) added later. HAPPy will be able to employ various different programs for each stage of the process, with an emphasis on using CCP4 software. Current modules include SHELXD for substructure determination, MLPHARE, PHASER and BP3 for phasing, followed by PIRATE for phase improvement. In the future there will be BUCCANEER and COOT modules for model building. HAPPy is designed to integrate with CCP4i and other automation projects, *e.g.* DNA/XIA, through the use of well-defined APIs and data exchange protocols. HAPPy is currently under development, with priorities being rigorous testing to assess and improve the scoring, decision making and crucial parameters.