Tracing polypeptide chains in electron-density maps

Tom Terwilliger
Los Alamos National Laboratory
Rapid chain-tracing for evaluation of map quality

(armadillo repeat of β-catenin, 369 residues, 23 sec)
Points in high density

(s-hydrolase, PDB entry 1A7A)
Move points to ridgelines

(s-hydrolase, PDB entry 1A7A)
Find possible $C_\alpha$ pairs
(3.8 Å apart, high density between, points near line)
Find possible $C_{\alpha}$ trimers

(Pairs sharing $C_{\alpha}$; $110^\circ$ angle; points near line extending from vertex)
$C_\alpha$ tracing
(s-hydrolase, PDB entry 1A7A)
$C_\alpha$ tracing
(mevalonate kinase, PDB entry 1KKH, 9 sec)
C$_\alpha$ tracing
(1038B, PDB entry 1LQL, 114 sec)
Using secondary structure content to evaluate map quality
The PHENIX Project

Lawrence Berkeley Laboratory
Paul Adams, Ralf Grosse-Kunstleve, Pavel Afonine, Nat Echols, Nigel Moriarty, Jeff Headd, Nicholas Sauter, Peter Zwart

Los Alamos National Laboratory
Tom Terwilliger, Li-Wei Hung

Duke University
Jane & David Richardson, Vincent Chen, Chris Williams, Bryan Arendall, Laura Murray

Cambridge University
Randy Read, Airlie McCoy, Gabor Bunkoczi, Rob Oeffner

An NIH/NIGMS funded Program Project