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Higher-Quality Structures Assured at SECSG. W. Tempel¹, W.B. Arendall III², J.S. Richardson², W. Zhou¹, S. Wang², I.W. Davis², Z.J. Liu¹, L. Chen¹, L. Deng¹, J.P. Rose¹, W.M. Carson³, M. Luo³, D.C. Richardson², B.C. Wang¹, Southeast Collaboratory for Structural Genomics, ¹Univ. of Georgia, Athens, GA 30602, ²Duke Univ. Medical Center, Durham, NC 27710, ³Univ. of Alabama, Birmingham, AL 35294.

The collection of highly accurate diffraction data and model validation at all stages of refinement have been integrated at SECSG to ensure high-quality structural-genomics structures. A carefully designed and executed diffraction experiment is fundamental in Direct Crystallography, one of the objectives of our center.

In our approach, refinement is initiated with a chemically reasonable model. Errors are detected and repaired, as needed, along the pathway of refinement using the all-atom contact analysis tool MolProbity, which also contains updated Ramachandran and side chain rotamer criteria.

The effectiveness of this integrated validation/refinement approach in obtaining higher-quality structural models has been evaluated. While control structures from SECSG performed comparable to typical PDB models, structures from SECSG with MolProbity validation are of higher quality than the control structures.

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