Beautifying 3D-SHOTGUN models

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C-alpha, unrefined models were automatically generated for all targets using the 3D-SHOTGUN server. 3D-SHOTGUN assembles hybrid, C-alpha-only, unrefined models that can be an excellent starting point for refinement.

For CASP, we refined the 3D-SHOTGUN models using either Honig's nest or Keasar's beautify refinement programs. The resulting models are full-atom, physically valid models. Large tests from LiveBench indicate that the performance of these refinement programs in combination with 3D-SHOTGUN, is superior to that obtained by other refinement programs previously used. The MaxSub scores of the resulting models are on average almost identical to those obtained for the original 3D-SHOTGUN models. Thus, this procedure achieves two goals: accuracy and beauty. The first goal is achieved because 3D-SHOTGUN produces excellent unrefined models. The second goal is achieved because the refinement, without decreasing accuracy, produces physically valid, full-atom models. For verification purposes, the resulting full-atom models were assessed using the new MQAP-CONSENSUS method developed for MQAP-CAFASP (www.cs.bgu.ac.il/~dfischer/CAFASP4). The MQAP-CAFASP scores of our refined models were also compared to models produced by the CAFASP servers.

Results from the evaluation of the nearly 30 CASP6 targets whose structures have been released indicate that the beautified 3D-SHOTGUN models submitted to CASP6 are of relatively high quality: their total MaxSub score is higher than that obtained by the best CAFASP4 servers and meta-servers.