

W0450

Finding the Best Composite Model from Multiple Sources. Dusan Turk¹, Maksymilian Chruszcz², Marcin Cymborowski², Wladek Minor², Zbyszek Otwinowski³, ¹Jozef Stefan Inst., Ljubljana, Slovenia, ²Univ. of Virginia, Charlottesville, VA, ³Univ. of Texas, Dallas, TX.

Molecular models generated by automated chain tracing are sensitive to resolution of maps, their contouring level, software and even to grid spacings used, which means that the generated models resulting from single runs are different. The observation is that a single model may not be the best everywhere especially when only medium resolutions phases are available. Therefore it makes sense to generate an ensemble of models, superimpose them and select fragments, which define the best trace and merge them into the unique, composite model.

For this purpose a procedure has been developed in MAIN 2006, which can generate the best trace from a variety of molecular models. First all models are superimposed using crystal symmetry operators. Superimposed residues are assigned into clusters, which build overlapping chain traces. These get secondary structures assigned. The best helix and beta strand traces are found by choosing the smaller number of fragments, which build the longest secondary structure segment. All other connectivities between the clusters in the secondary structure region are then discarded. In the next step the connecting segments between the ends of secondary structure elements and the chain termini are being found. Cross connections between the connecting segments are removed considering the chain directionality and reduction of cross segment connections. (Each knot may have up to two outgoing branches.) The trace of connecting segments is then optimized by a search procedure, which finds the best trace of overlapping fragments in the region. The resulting unique trace through the residue clusters is then converted into a single chain trace, energetically minimized and used for further model building.

For software see "<http://www-bmb.ijs.si/>".