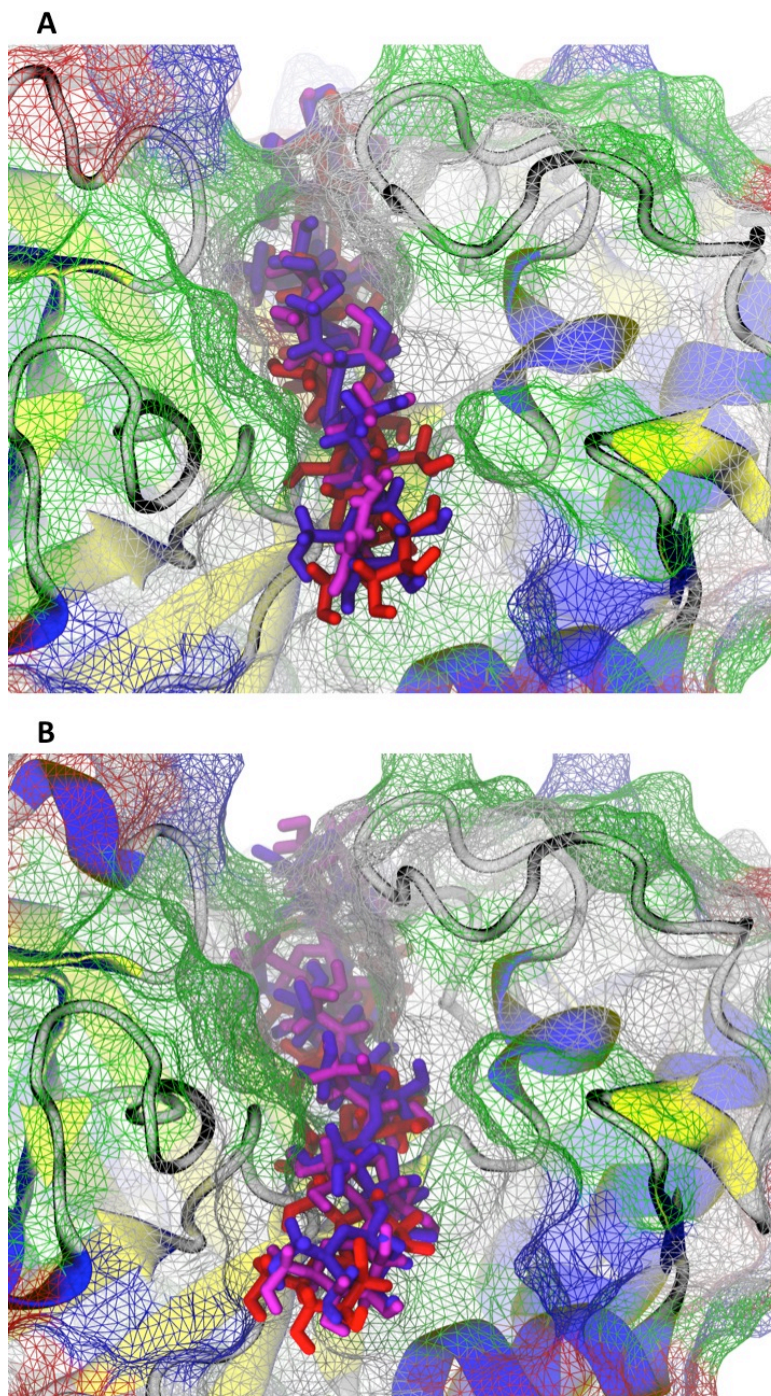


Additional file 1

Supporting Figure 1: Illustration of Man5B with cellohexaose (A) and mannohexaose (B) in the catalytic pocket after docking and initial equilibration. As template for docking of the hexasaccharide substrates we used the protein data bank structures [PDB:1CEN] (hexasaccharides shown in blue) and [PDB:3AMG] (hexasaccharides shown in magenta and in red). For each of the three different templates the cellohexaose structures were stable and in similar conformations. In case of mannohexaose, docking and initial equilibration resulted also in three similarly stable conformations, albeit with slightly different geometries compared to those seen in the cellohexaose. The catalytic pocket of Man5B is mainly hydrophobic as represented by the white color in the triangulated surface mesh. In the triangulated surface mesh the color green represents hydrophilic regions while blue represents positively charged groups and red negatively charged groups.