Supplemental Information

ConTemplate Suggests Possible Alternative

Conformations for a Query Protein

of Known Structure

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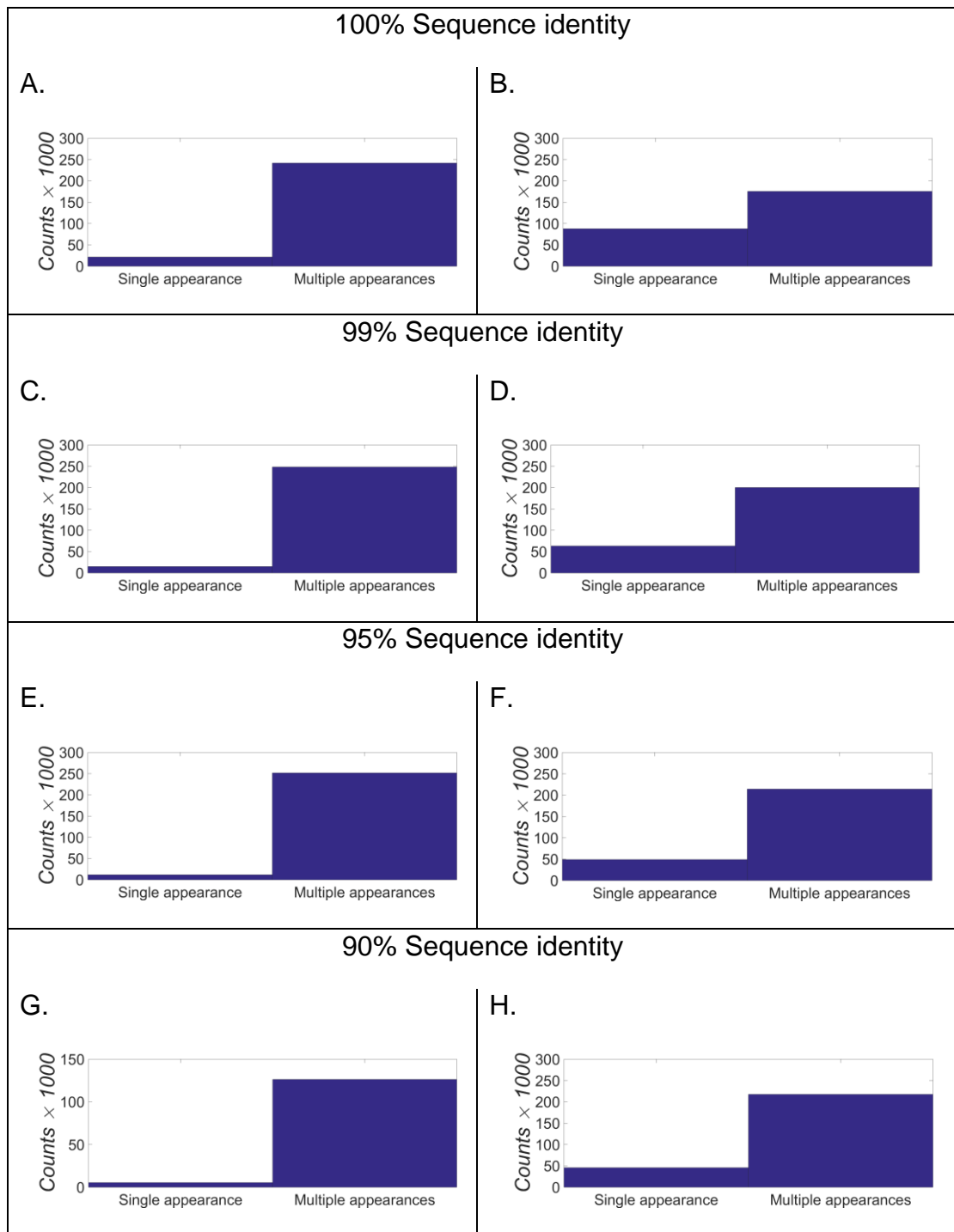
Figure S1, related to Figure 1. Most of the polypeptide chains in the PDB appear in multiple entries. **A.** The number of chains that appear only once vs. these appearing two times or more in the PDB (100% sequence identity and full coverage). **B.** Same as "A", excluding multiple appearances within the same PDB entry. **C & D.** Same as "A" and "B" for 99% sequence identity. **E & F.** Same as "A" and "B", for 95% sequence identity. **G & H.** Same as "A" and "B", for 90% sequence identity.

Table S1, related to Figure 2. Proteins that share a similar structure usually belong to the same ECOD X-group, and have similar functions. We ran an all-vs.-all structure alignment between the set of 246 proteins with up to 80% sequence identity in 516 alternative conformations, each of them has at least two conformations that superimpose to each other with RMSD of 4Å or more. The rows in the table describe pairs of proteins in that set that had a structurally-similar conformation. The first batch shares also at least one other conformation with each other. For each pair, ECOD's X-group annotation and the GO annotations are indicated. In the vast majority of cases, the proteins share the same X-group and function.

Movie S1, related to Figure 5. A pathway between the query and target conformations of the ribose binding protein. The query is the ribose-bound conformation, and the target is the ligand-free conformation of this protein. The pathway is the shortest path from the query to the target, found using Cytoscape. There are 5 frames in the movie, each displaying a single structure: the query conformation, 3 models obtained by ConTemplate, and the target conformation. The RMSD between two structures shown in consecutive frames is 2.5Å or less.