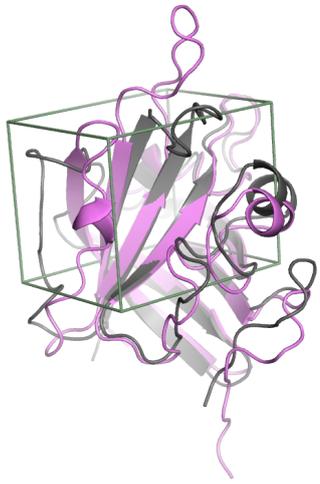
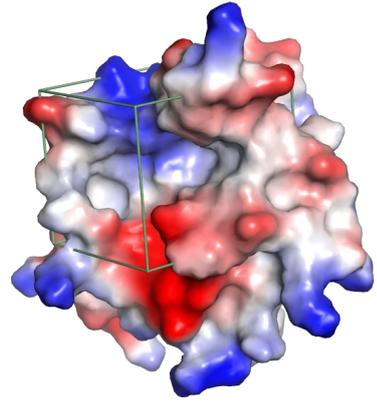
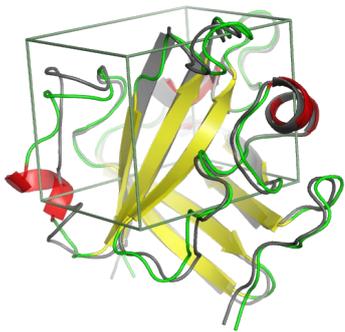
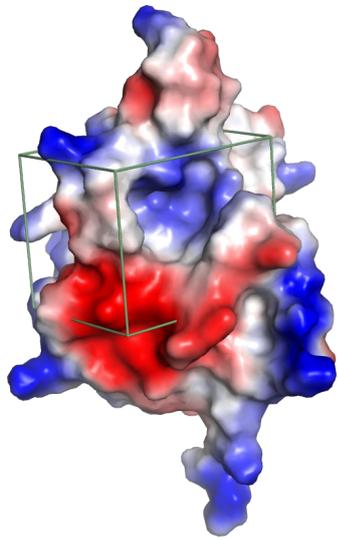


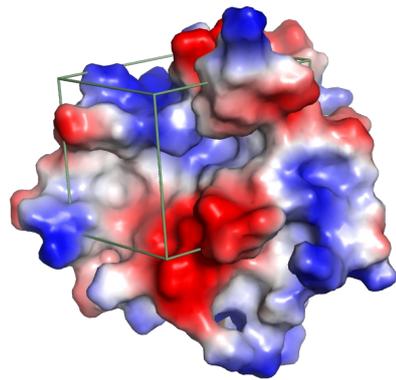
A

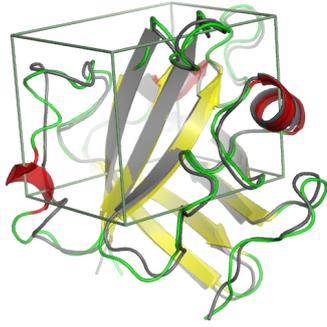


B

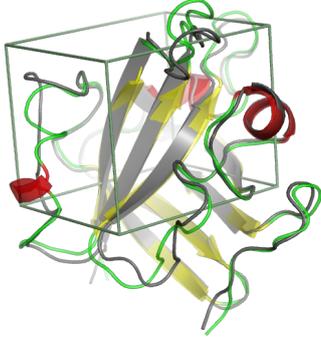
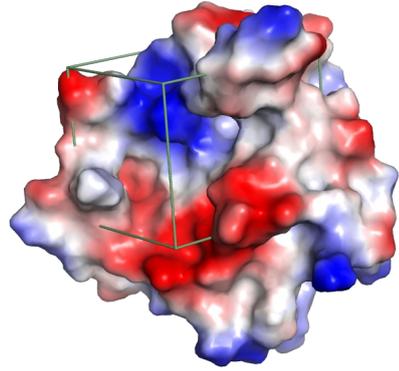


C

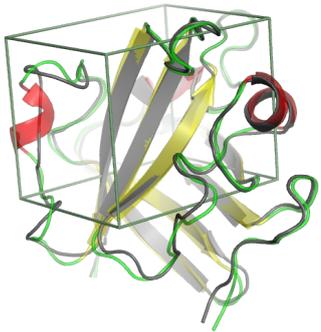
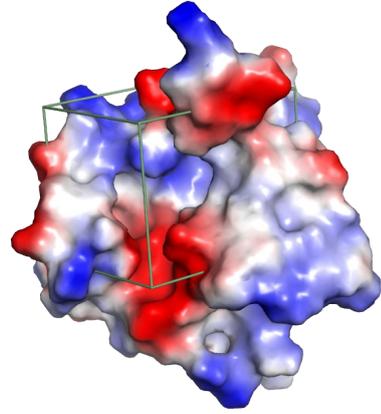




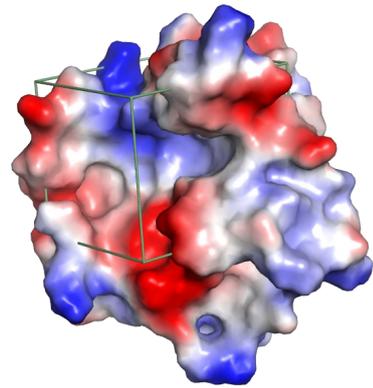
D



E



F



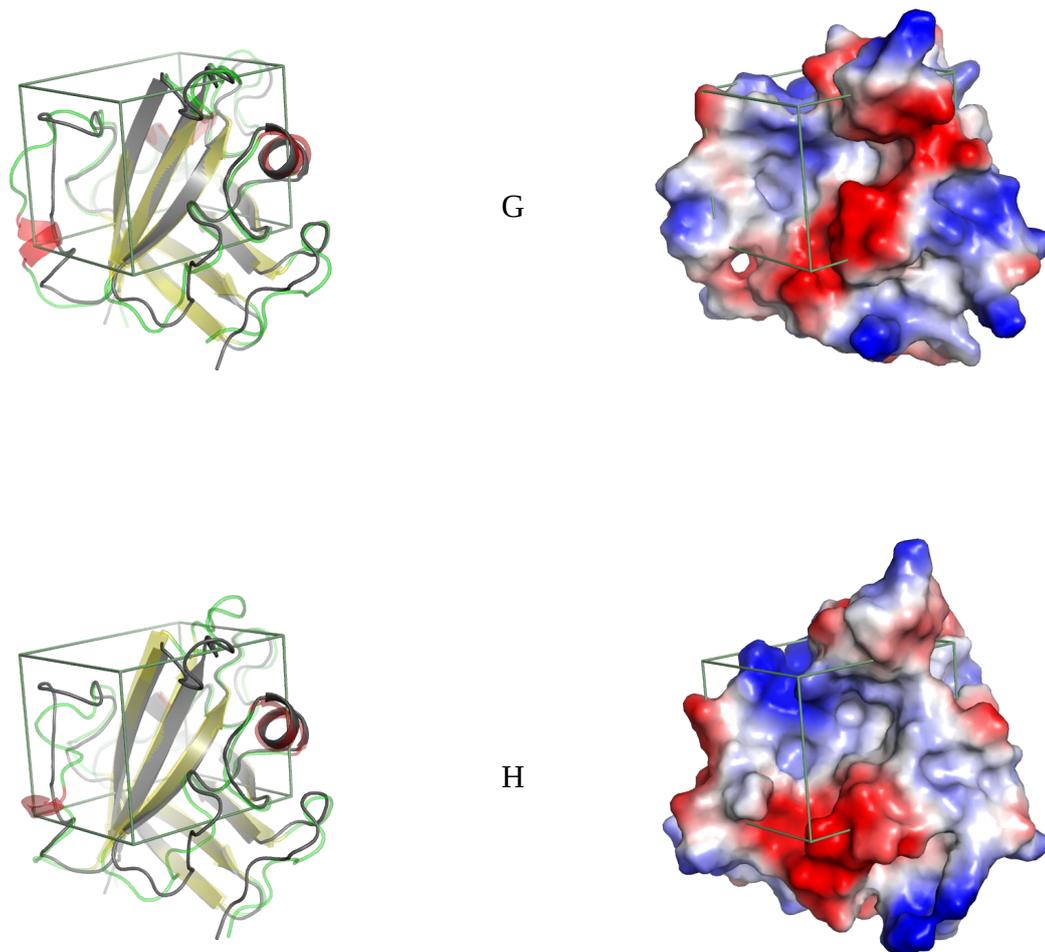


Figure S1. Depiction of the grid bounding box used for docking for each of the protein structures used: A – PDB:1T2W (the main template), B – PDB:2KID, C – Cluster #1, D – Cluster #2, E – Cluster #3, F – Cluster #4, G – Cluster #5, H – Cluster #6. Ribbon models (left column) are superimposed over PDB:1T2W geometry for reference which is shown in grey.