Structural Variation of BRD4-BD1 Complexes – Supporting Information

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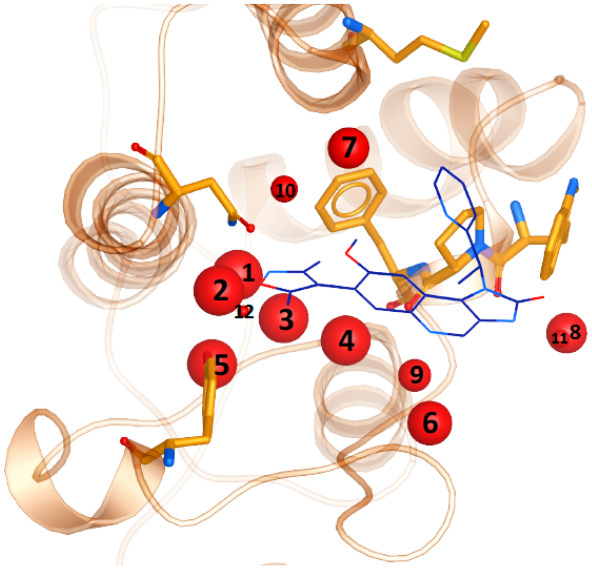
1) Active Site Water Molecules: Crystallographic water molecules (red) in the binding pocket of BRD4-BD1 (orange). The size of the spheres indicate the extent of their conservation across 101 crystal structures. For perspective, a small molecule binder (PDB 3ZYU) is shown in blue. A CSV file has been provided with a full list of PDB codes and the presence of active site crystallographic water molecules in each.



2) Ligands from 101 crystal structures of BRD4-BD1 complexes were docked against structure PDB 4BJX. To compare the two setups, the RMSD values between the docked poses and the crystallographic poses were calculated. The figure below shows the RMSD distributions between the two data sets.