To verify the accuracy of estimated hydrated protein sizes, we also calculate the radius of gyration based on X-ray crystal structures published in the protein data bank. In Table 1, we present the geometric radius of gyration defined as

$$R_g^2 = \frac{1}{n}\sum_{i=1}^{n}[(x_i - x_c)^2 + (y_i - y_c)^2 + (z_i - z_c)^2] \quad (28)$$

where n is the total number of atoms, $x_c = (\sum_{i=1}^{n} x_i)/n$, $y_c = (\sum_{i=1}^{n} y_i)/n$, $z_c = (\sum_{i=1}^{n} z_i)/n$, and (x_i, y_i, z_i) are the coordinates for atom i. In eq 28, we sum over all atoms except water that are identified in the protein data bank. We have checked the effect of including hydrogen atoms on the geometric radius of gyration. This is accomplished by using the H-Build facility in CHARMM.[59] We find that adding hydrogen atoms does not significantly change the radius of gyration. For example, the geometric radius of gyration for myoglobin after including the hydrogen atoms is 15.5 Å, which is only slightly larger than the 15.2 Å obtained without hydrogen atoms. It is found that $R_g = 15.2$ Å for myoglobin (PDB ref no.:, 1MBS) and 14.3 Å for ribonuclease (PDB ref no., 3RN3). These radii of gyration, R_g, plus the diameter of water, 3 Å, are very close to the estimated hydrated protein radius, R'_p. However, the radius of gyration for conalbumin (PDB ref no.: 1OVT) is 29.5 Å, which is about the same as R'_p (30 Å). Thus, the size of hydrated conalbumin is underestimated. As Table 1 shows, using $R'_p = R_g + 2R_W = 32.5$ Å for conalbumin improves the already good agreement between theoretical predictions and experimental data. Thus, R_g+2R_W is a more accurate way to estimate the size of a hydrated protein if R_g is known.