Erratum: "Anisotropic coarse-grain Monte Carlo simulations of lysozyme, lactoferrin, and NISTmAb by precomputing atomistic models" [J. Chem. Phys., 161, 094113 (2024)]

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The authors initiate a correction to Hatch *et al.*[1] If the particles are of the same type, particle swap symmetry was improperly applied by limiting the azimuthal angle to values of 0 to π by choosing the reference particle based on the azimuthal angle when only the first particle was considered the reference particle. This correction simply does not use particle swap symmetry and allows azimuthal angles in the full range of 0 to 2π. The correction improves the coarse-grained (CG) model results by bringing them closer to the all-atom (AA) model results. Although this correction resulted in minor changes to Figs. 4-7, 9, 13 and 14 of the original article, now shown in Figs. 1-7, there is no qualitative change to the data trends or conclusions of the original article.[1] In addition, a typo was also discovered in the caption of Fig. 14 of the original article[1] for the pH of the Fab fragment, which was pH 3 but erroneously reported as pH 6. The corrected methodology is available in the open-source software FEASST version 0.25.18.[2]

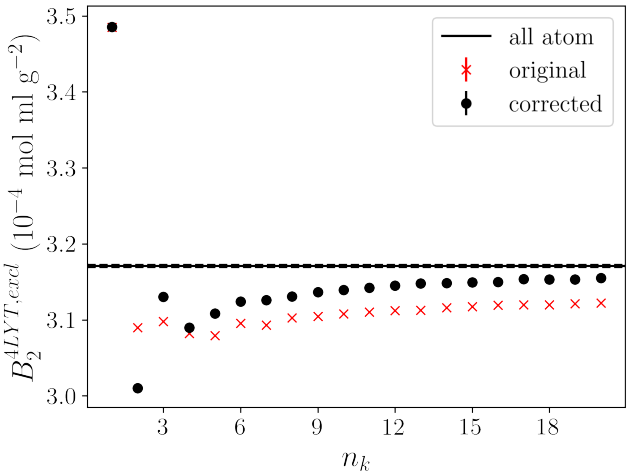

FIG. 1: The B_2 of lysozyme (PDB ID 4LYT) with only excluded volume interactions as a function of the number of orientations per 180 degrees, n_k for the CG model. Error bars are the standard error of the mean and are smaller than the symbols. The solid horizontal line shows the average of the AA value, while the dashed lines outline the range of uncertainty from the standard error of the mean. The red X's show the results from Fig. 4 of the original article,[1] while the black circles show the corrected results.

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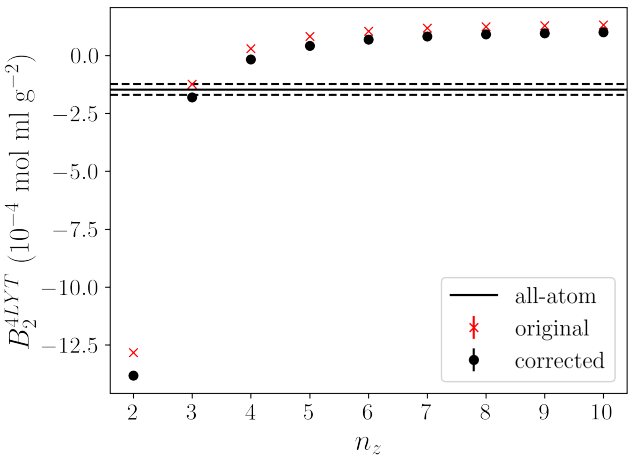

FIG. 2: The B_2 of lysozyme (PDB ID 4LYT at pH 6) as a function of the number of distances, n_z, per orientation with $n_k = 12$. Error bars are the standard error of the mean and are smaller than the symbols. The solid horizontal line shows the average of the AA model value, while the dashed lines show ± the standard error of the mean. The red X's show the results from Fig. 5 of the original article,[1] while the black circles show the corrected results.

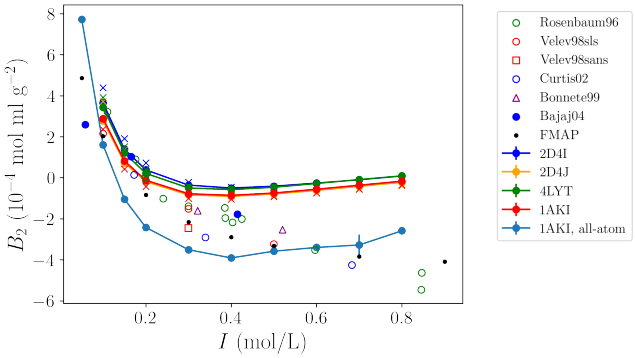

FIG. 4: The B_2 of lysozyme at pH 4.5 from previously published experimental data[3–7] are shown with open symbols and the blue circle. The CG models for various PDB IDs (4LYT, 1AKI, 2D4I, 2D4J) as a function of the ionic strength, I, with $n_k = 12$, $n_z = 7$ are shown by the lines. AA values for 1AKI are shown in purple and the FMAP[8] results with a different protonation state are also shown by the black dots. Error bars are standard error of the mean and may be smaller than the symbols. The X's show the results from Fig. 7 of the original article,[1] while the circles with connecting lines show the corrected results.

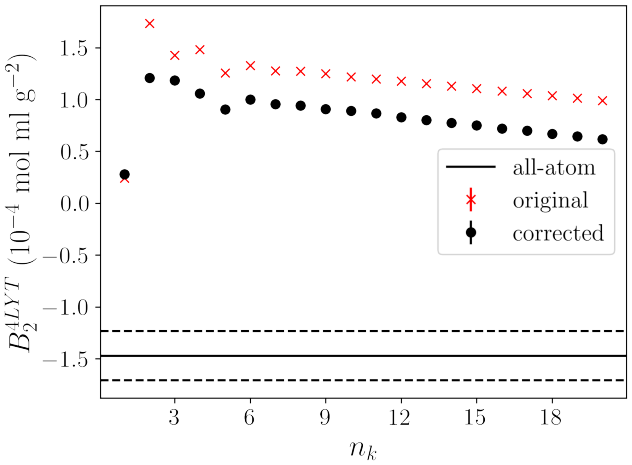

FIG. 3: The B_2 of lysozyme (PD ID 4LYT at pH 6) as a function of the number of orientations per 180 degrees, n_k, for $n_z = 7$. Error bars are the standard error of the mean and are smaller than the symbols. The solid horizontal line shows the average of the AA model value, while the dashed lines show ± the standard error of the mean. The red X's show the results from Fig. 6 of the original article,[1] while the black circles show the corrected results.

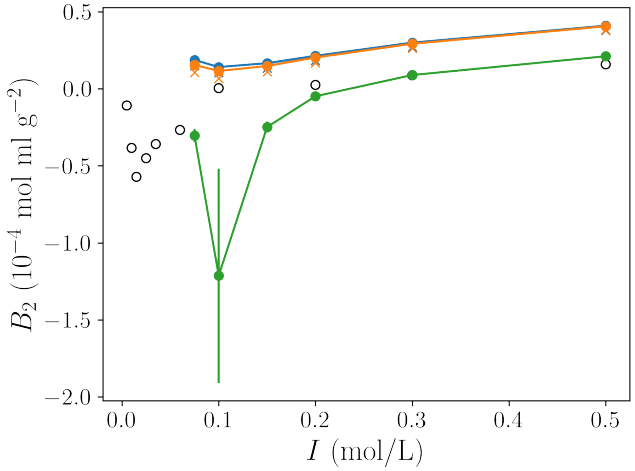

FIG. 5: The B_2 of lactoferrin (PDB ID 1BLF) at pH 7 with previously published experimental data shown by the open circles,[9] and the CG models as a function of the ionic strength for different orientational resolution, closed circles (blue) $n_k = 10$ and (orange) $n_k = 12$. AA values are shown in green, and the results from Fig. 9 of the original article[1] are shown with X's. Error bars are standard error of the mean and may be smaller than the symbols.

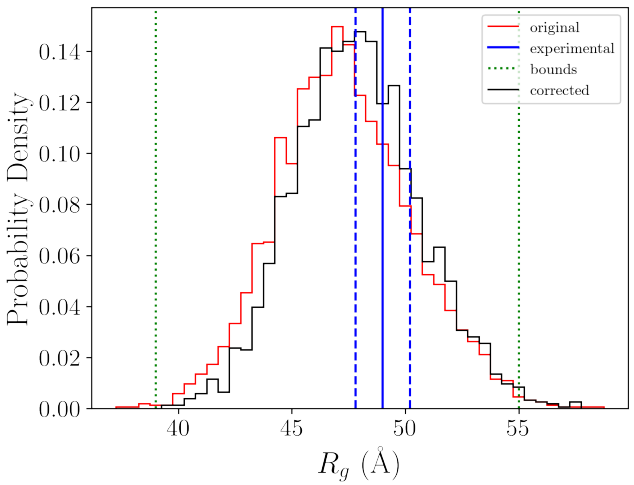

FIG. 6: The probability of the radius of gyration of the CG model of the NISTmAb for pH= 6, $I = 0.15$ mol/L, $n_k = 12$, $z = 7$ is shown by the histograms with 0.5 Å resolution. The red histogram shows the results from Fig. 13 of the original article,[1] while the black histogram shows the corrected results. The solid vertical line is the experimental value of 49 Å, and the dashed lines show the experimental standard deviation of 1.2 Å.[10,11] The dotted vertical lines correspond to the lower and upper limits of 39 and 55 Å from previous MC methods.[12] The corrected average from the CG simulations in this work was 47.86 Å with a standard error of the mean of 0.06 Å. The average of the corrected results is roughly 0.5 Å closer to the experimental value than the original results.

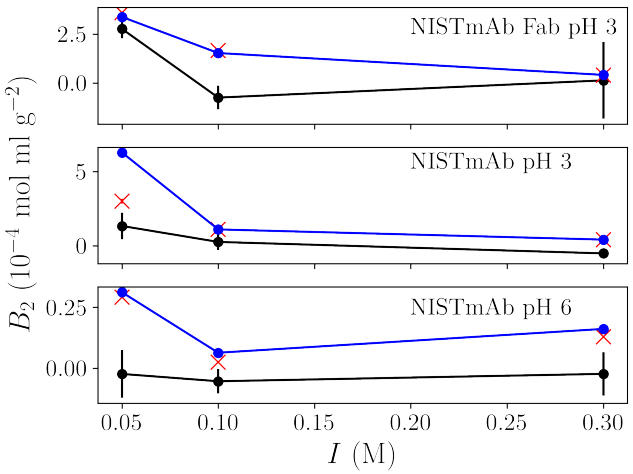

FIG. 7: (top) Second virial coefficient, B_2 of the Fab domain of the NISTmAb from (black) previous scattering experiments[13] and (blue) MSMC with a CG model, $n_k = 12$, $n_z = 7$, pH 3. Red X symbols show the original results from Fig. 14 of the original article.[1] (middle) B_2 of the entire NISTmAb for (solid lines with a circle) with pH 3 and (bottom) pH 6. Error bars for simulations are standard error of the mean and may be smaller than the symbols, and error bars for experiments are as previously reported.[13]

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