Model-potential-free analysis of small angle scattering of proteins in solution: insights into solvent effects on protein-protein interaction

Tomonari Sumi, Hiroshi Imamura, Takeshi Morita, Yasuhiro Isogai, and Keiko Nishikawa

Electronic Supplementary Information

A procedure for the model-potential-free analysis

The values of $\hat{h}'(q)$ for $q \leq q_{\mathrm{h}}$ in Eq. (4) are fixed as $\hat{h}_{\mathrm{exp}}(q) = \left[S_{\mathrm{exp}}(q) - 1\right] / n_0$ during the iterative calculation for solving the integral equation, whereas the values of $\hat{h}'(q)$ for $q > q_{\mathrm{h}}$ in Eq. (4) are updated using the Fourier transform of $h(r)$ calculated using Eq. (2). The parameter q_{h} is the maximum value of a scattering vector for which the experimental $S_{\mathrm{exp}}(q)$ is available for use. The prime of $\hat{h}'(q)$ indicates the Fourier-transformed $h(r)$ after replacement with $\hat{h}_{\mathrm{exp}}(q)$ for $q \leq q_{\mathrm{h}}$.

An initial guess in the iterative calculation is given by the following:

$$\hat{c}(q) = \hat{c}_{\mathrm{HS}}(q), \tag{A1}$$

$$\hat{\gamma}_{\mathrm{s}}(q) = \hat{\gamma}_{\mathrm{s}}^{\mathrm{old}}(q) = 0, \tag{A2}$$

$$\hat{h}^{\mathrm{old}}(q) = \hat{h}_{\mathrm{HS}}(q), \tag{A3}$$

$$\hat{h}'(q)=\begin{cases} \hat{h}_{\mathrm{exp}}(q) & q \le q_{\mathrm{h}} \\ \hat{h}_{\mathrm{HS}}(q) & q > q_{\mathrm{h}} \end{cases}, \tag{A4}$$

where $\hat{h}_{\mathrm{HS}}(q)$ is obtained from the hard-sphere reference system.

The following iterative calculation is continued until the absolute difference between $\hat{h}(q)$ and $\hat{h}^{\mathrm{old}}(q)$ becomes less than a threshold.

1. $\hat{c}_{\mathrm{ex}}(q)=\hat{c}(q)-\hat{c}_{\mathrm{HS}}(q)$. (A5)

2. $\hat{c}(q)=\hat{h}'(q)-\left[\hat{\gamma}_{\mathrm{s}}(q)-\hat{c}_{\mathrm{ex}}(q)\right]$. (A6)

3. $\hat{\gamma}_{\mathrm{s}}(q)=\hat{c}(q)/\left[1-n_0\hat{c}(q)\right]-\hat{c}_{\mathrm{HS}}(q)$. (A7)

4. $\hat{\gamma}_{\mathrm{s}}(q)=a\hat{\gamma}_{\mathrm{s}}(q)+(1-a)\hat{\gamma}_{\mathrm{s}}^{\mathrm{old}}(q)$, where a is the dumping parameter.(A8)

5. $\hat{\gamma}_{\mathrm{s}}^{\mathrm{old}}(q)=\hat{\gamma}_{\mathrm{s}}(q)$. (A9)

6. $h(r)=\begin{cases} \exp\left[\gamma_{\mathrm{s}}(r)+B(r)\right]-1 & r > d_{\mathrm{HS}} \\ -1 & r \le d_{\mathrm{HS}} \end{cases}$. (A10)

7. If the difference between $\hat{h}(q)$ and $\hat{h}^{\mathrm{old}}(q)$ becomes less than the threshold, go to step 8 (outside the loop of the iterative calculation); otherwise, we update as $\hat{h}^{\mathrm{old}}(q)=\hat{h}(q)$ and $\hat{h}'(q)=\hat{h}(q)$ for $q > q_{\mathrm{h}}$, go back to step 1.

8. $S(q)$ is calculated as $S(q)=1+n_0\hat{h}(q)$.

A comparison between the experimental raw *S*(*q*) and its smoothed *S*(*q*)

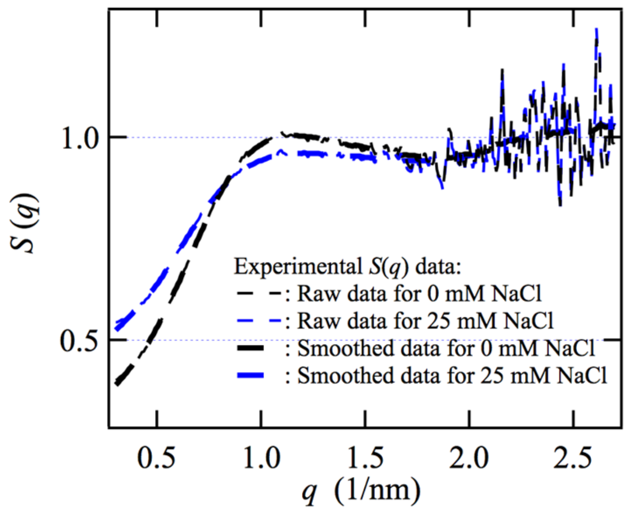

Fig. S1 The experimental raw structure factor $S_{\exp}(q)$ that was directly obtained from dividing the raw scattering intensity $I_{\exp}(q)$ for 10 wt% dense lysozyme solutions by a form experimental factor $P_{\exp}(q)$ and its smoothed $S_{\exp}(q)$. The form factor $P_{\exp}(q)$ was determined from the scattering intensity $I_{\exp}(q)$ for 0.26 wt% diluted lysozyme solution via $P_{\exp}(q)=I_{\exp}(q)-0.0135\times I_{\exp}(q=0)$. Here, $I_{\exp}(q=0)$ is an extrapolation value of $I_{\exp}(q)$ toward the low-q limit with a Gaussian function. The factor $0.0135\times I_{\exp}(q=0)$ is a base line correction we introduced so that the values of $S(q)$ should not deviate from 1 at high-q values. In order to obtain the smoothed $S(q)$ data as shown in Fig. S1, we applied the Savitzky–Golay smoothing to the experimental raw data of $S(q)$.

A comparison between experimental and theoretical scattering intensities

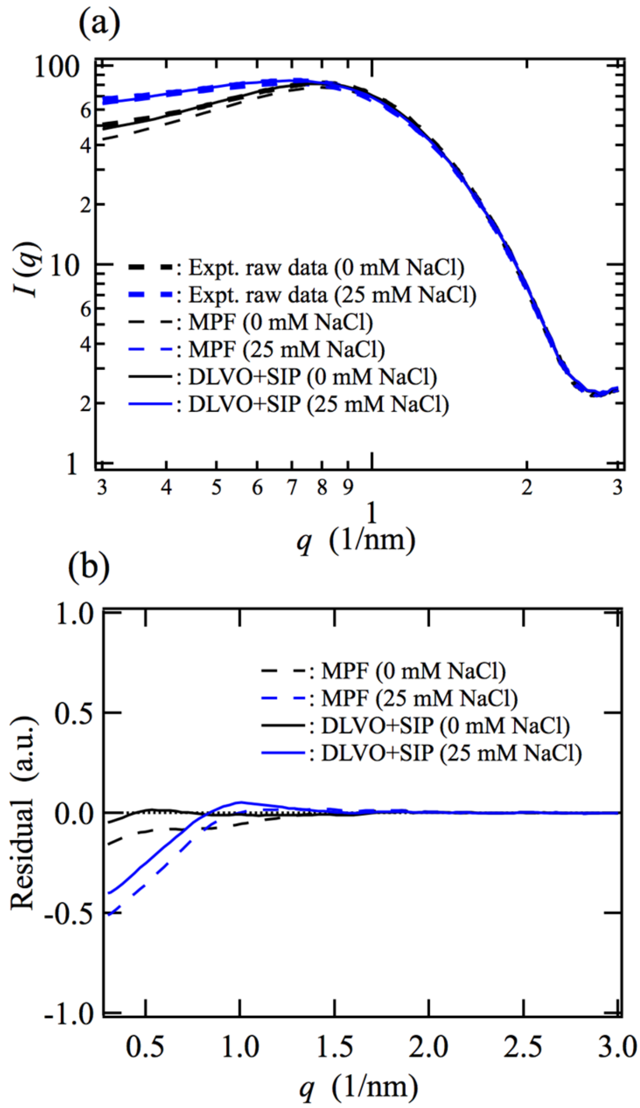

Fig. S2 (a) The experimental raw scattering intensity $I(q)$ and the theoretical $I(q)$ that was obtained from the product of the theoretical structure factor $S(q)$ and the form factor $P(q)$. (b) The differences between the theoretical $I(q)$ and the experimental raw $I(q)$.