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Supporting information for article:

Size-refocusing fitting of small-angle X-ray scattering from polydisperse nanoparticles for shape determination
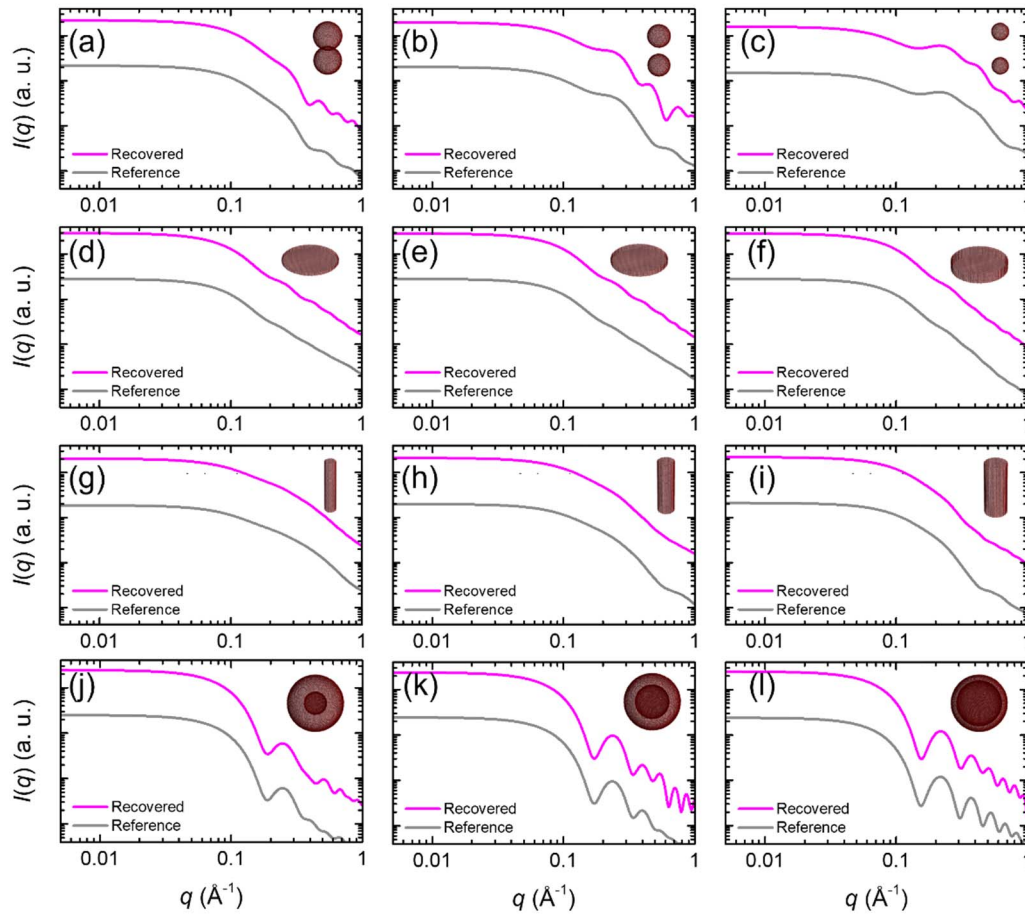
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S1. Supplementary figures

Figure S1 The corresponding SAXS intensity profiles calculated from the recovered PDDF profiles (pink curves) and reference PDDF profiles (gray curves) presented in Figure 5. The two SAXS curves in each panel were offset for easy visualization.
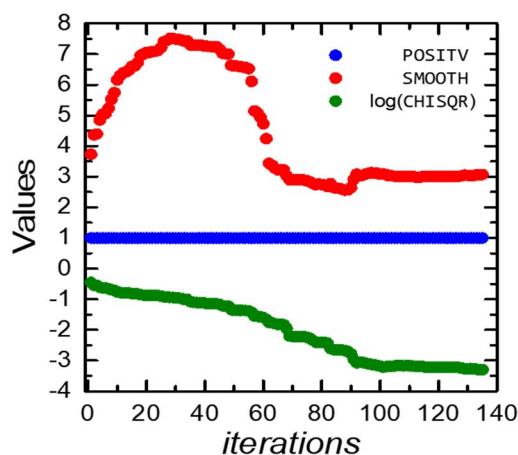
Figure S2 The evolution of values of each term in the goal function as a function of the number of iterations during the fitting procedure presented in Figure 6.
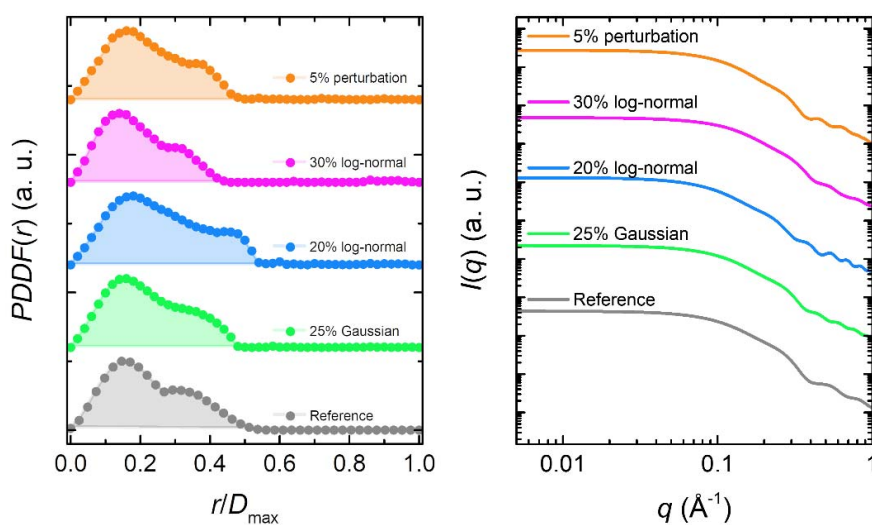

Figure S3 (a) The recovered $\hat{P}_0(r/D_{\max})$ ($D_{\max} = 80$ Å) of dimer particle ensembles presented in Figure 5(a) at different falsely given conditions: orange - 5% perturbation (noise) added to $P_{ens}(r)$; pink - given a $\sigma = 0.30$ (~30%) log-normal size distribution; blue: given a $\sigma = 0.20$ (~20%) log-normal size distribution; green - given a $\sigma = 0.25$ (25%) Gaussian size distribution. Gray curve represents the reference curve calculated by the voxel model. (b) The corresponding SAXS intensity profiles calculated from the PDDF profiles presented in (a). The curves were offset for easy visualization.
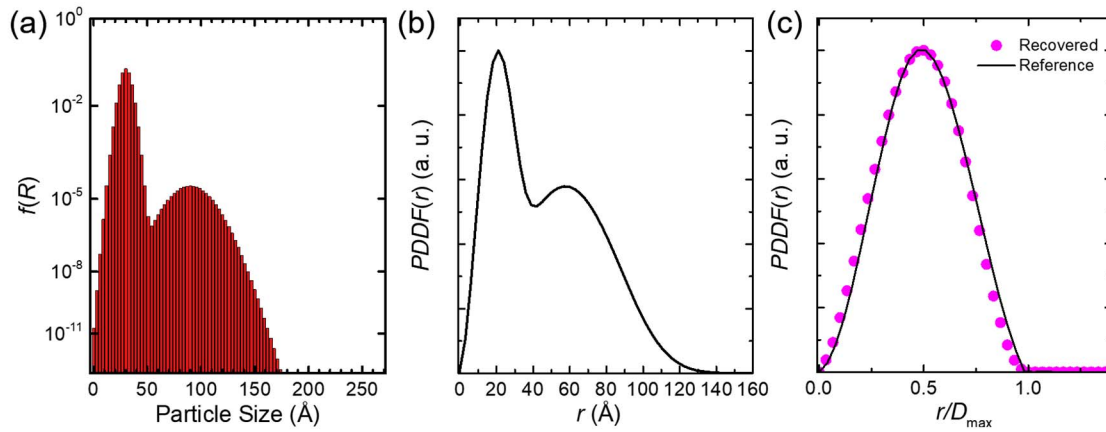
Figure S4 Refocusing the PDDF of spherical nanoparticle from a bimodal Gaussian size distribution. (a) Simulated size distribution consisting of two Gaussian distributions, with mean diameters of 30 Å and 90 Å, both exhibiting a standard deviation of 15%. The ratio of the respective particle numbers was set to 1:1000 to ensure comparable contributions of these two groups of nanoparticles to the PDDF. (b) The PDDF spherical nanoparticle ensembles with a bimodal Gaussian size distribution (c) The deconvoluted, size-refocused PDDF with the characteristic one-peak, symmetric feature of the spherical particle, compared to the reference.