Supporting Information

Modeling solution X-ray scattering of biomacromolecules using an explicit solvent model and the fast Fourier transform

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Table S1 The χ^2 values between the computed and experimental scattering intensities for the three benchmark proteins using different solvation shell thicknesses. The protein backbone restraint MD simulation trajectories are used to compute scattering intensities.

Thickness of solvation shell (nm)	Lysozyme	Myoglobin	RNase
0.5	0.560	5.605	0.647
0.7	0.616	6.078	0.735
1.0	0.990	3.804	0.882
1.5	1.087	4.107	0.977
2.0	1.248	5.260	0.775
2.5	1.032	7.172	0.677
3.0	2.256	5.972	1.287

Table S2 The χ^2 values of the computed scattering intensities calculated by the Waxsis server and our FFT-based method, compared with the experimental scattering intensities of the three benchmark proteins. Solvent shell thickness of 0.7 nm is used in computations. Instead of Equation (8), the χ^2 values are calculated by minimizing $\chi^2 = N_q^{-1}\sum_{i=1}^{N_q}\left[\left(I_{exp}(q_i) - f \cdot I_{cal}(q_i)\right)/\sigma(q_i)\right]^2$, which does not contain the free parameter *c*.

	Lysozyme	**Myoglobin**	**RNase**
Waxsis	0.765	9.776	1.063
FFT	0.602	5.649	0.753

Figure captions

Figure S1 The computed scattering profiles using the all-atom simulation trajectories by the Waxsis server and our FFT-based method, compared with the experimental scattering profiles after minimizing the χ^2 values using $\chi^2 = N_q^{-1}\sum_{i=1}^{N_q}\left[\left(I_{exp}(q_i) - f \cdot I_{cal}(q_i)\right)/\sigma(q_i)\right]^2$, which does not contain the free parameter *c*. Solvent shell thickness of 0.7 nm is used in computation

Figure S1