

Supporting Information

Implicit vs. Explicit Solvent models for Calculating X-ray Solution Scattering Curves

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Performance of XSoS-Implicit. As described in the main text, we examined the performance of XSoS-implicit for a total of nine proteins. In Figure S1, we show theoretical scattering curves calculated by XSoS-implicit, CRY SOL and FoXS for the following proteins: (1) xylanase,¹ (2) malate synthase,² (3) superoxide dismutase from *Alvinella Pompejana*,³ (4)

complement fragment C3b complex with extracellular fibrinogen binding protein (Efb) from *Staphylococcus aureus*,⁴ (5) immunoglobulin-like domains 1 and 2 of the protein tyrosine phosphatase LAR3,⁵ (6) glucose isomerase,⁶ (7) C-terminal domain of glycosyl hydrolase,⁷ (8) ketoreductase-enoylreductase didomain,⁸ and (9) dimeric PYR1-

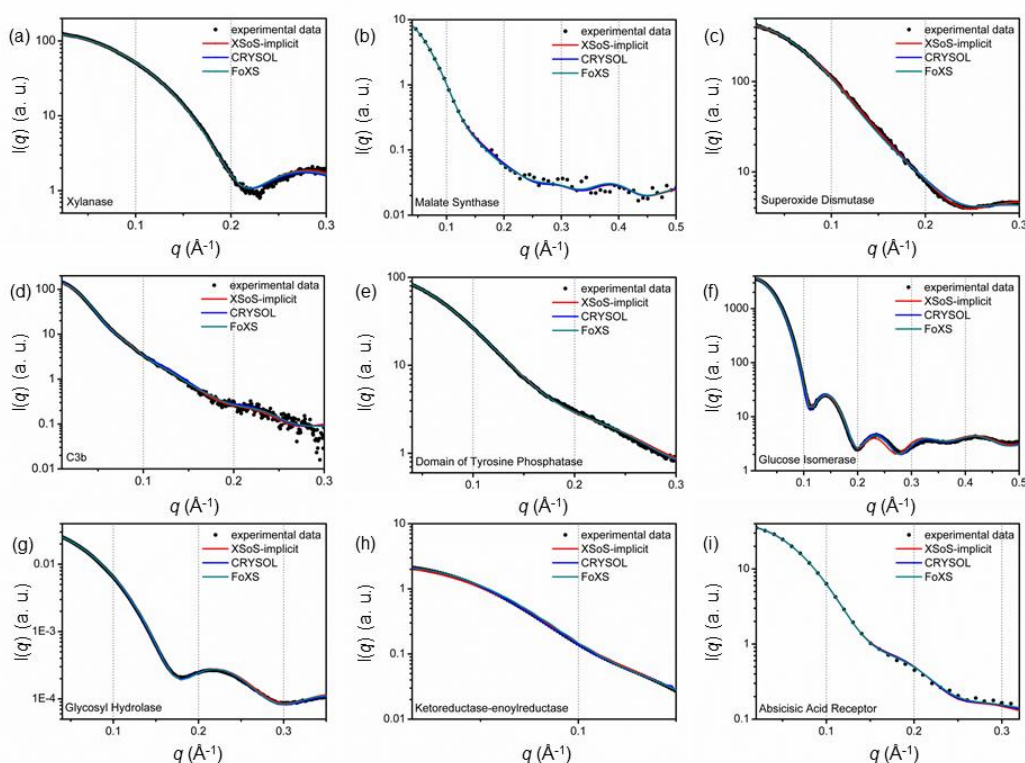


Figure S1 Static scattering curves of (a) xylanase, (b) malate synthase, (c) superoxide dismutase, (d) C3b fibrinogen binding protein (e) immunoglobulin-like domains 1 and 2 of the protein tyrosine phosphatase LAR3, (f) glucose isomerase, (g) C-terminal domain of glycosyl hydrolase, (h) ketoreductase-enoylreductase didomain, and (i) dimeric PYR1-abscisic acid complex calculated by the CRY SOL, FoXS and XSoS-implicit programs. The scattering curves calculated by XSoS-implicit (red line) well match the experimental scattering curves (black circles) as well as the theoretical scattering curves calculated by CRY SOL (blue line) and FoXS (green line).

abscisic acid complex.⁹ We can clearly see that the scattering curves calculated by XSoS-implicit well match the experimental scattering curves as well as the theoretical scattering curves calculated by CRY SOL and FoXS.

Performance of XSoS-explicit. As described in the main text, we examined the performance of XSoS-explicit for myoglobin and lysozyme. In Figure S2, we show theoretical scattering curves of lysozyme calculated by XSoS-explicit and EXCESS. It can be seen that the theoretical scattering curve calculated by XSoS-explicit well match the one calculated by EXCESS.

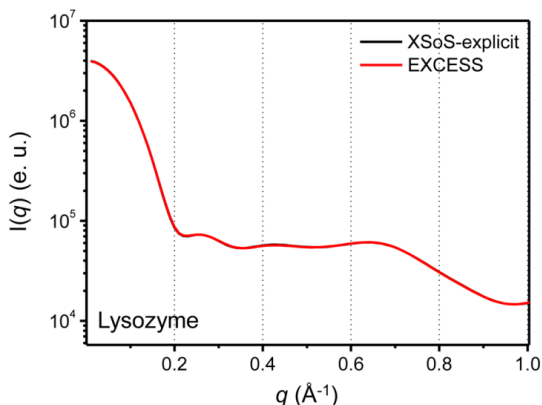


Figure S2 Static scattering curves of lysozyme calculated by XSoS-explicit (black line) and EXCESS (red line). The curves calculated by the two programs well match each other in the whole q range.

Convergence of scattering curves calculated by explicit solvent model. In the main text, we showed that the scattering curve calculated by XSoS-explicit converges into a curve of unique shape when using more than 500 MD snapshots. In order to confirm

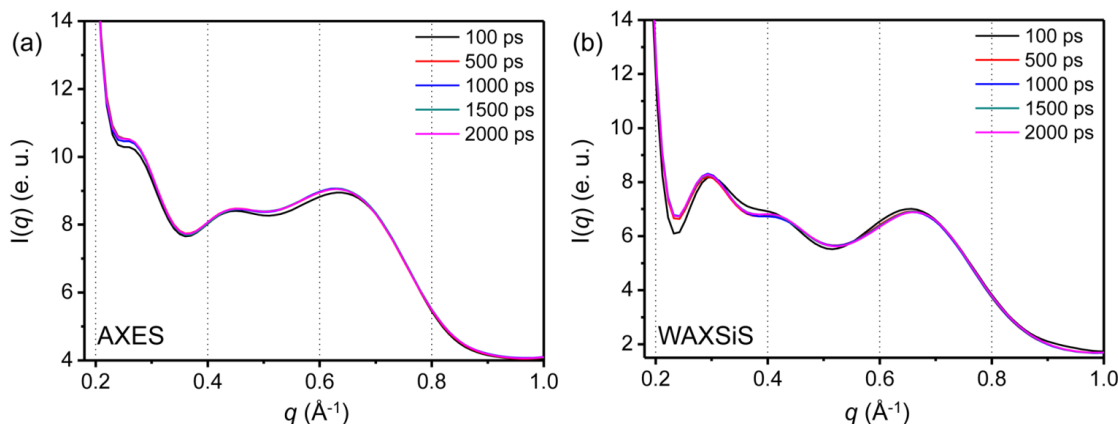


Figure S3 Scattering curves calculated using (a) AXES and (b) WAXSiS while varying the number of atomic coordinate sets to 100 snapshots (black line), 500 snapshots (blue line), 1000 snapshots (green line), 1500 snapshots (purple line) and 2000 snapshots (yellow line).

whether this finding is general for the explicit solvent model, we checked the convergence behavior with other explicit solvent-model programs, AXES and WAXSiS. As can be seen in Figure S3, the calculated scattering curve converges into a unique curve when the number of solvent degrees of freedom is over 500 snapshots for both AXES and WAXSiS.

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