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Supporting information for article:

Internal protein motions in molecular-dynamics simulations of Bragg and diffuse X-ray scattering

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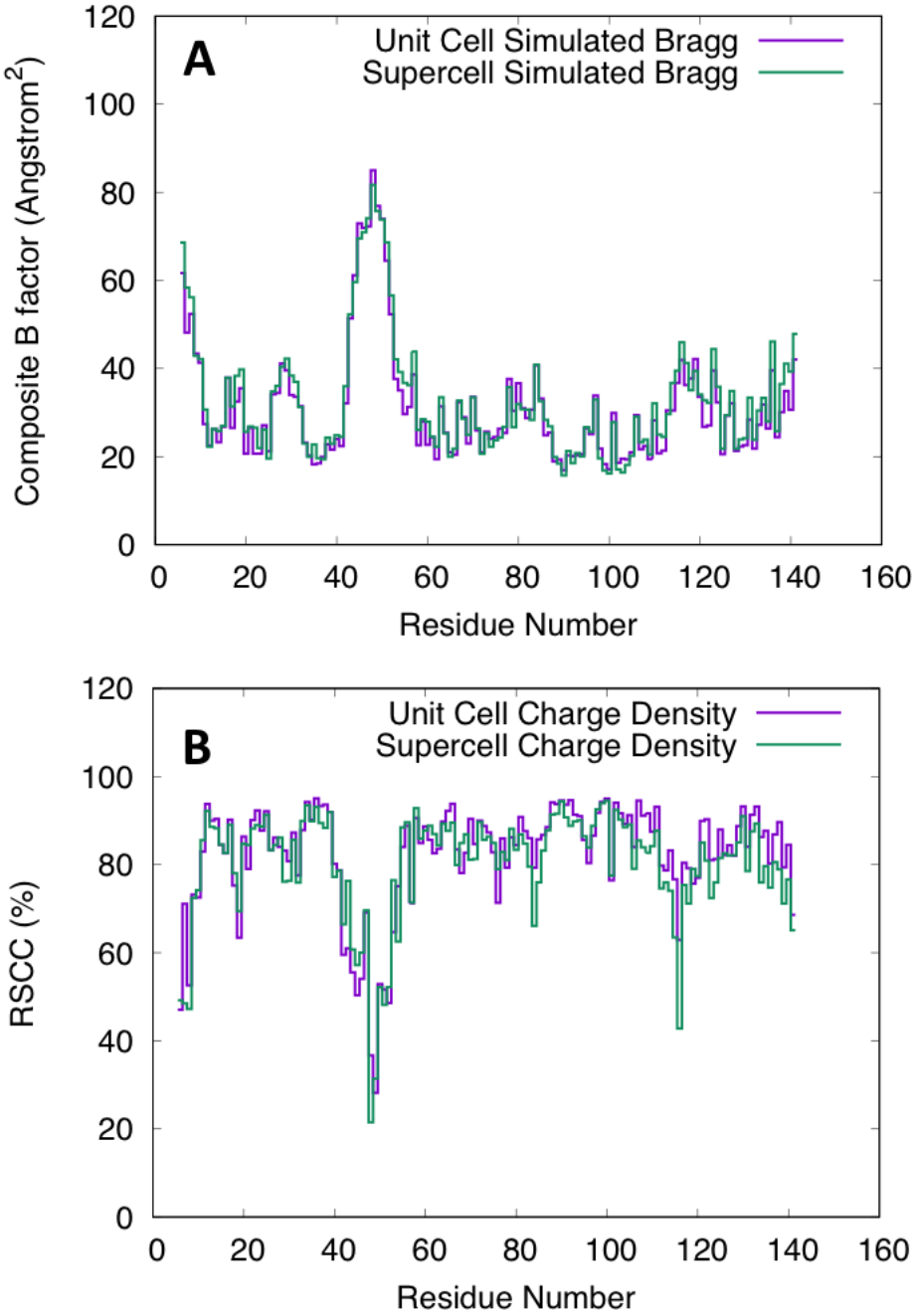

Figure S1 Comparison of Bragg analysis results for the unit cell vs. supercell simulations. (A) Residue-wise comparison between the B factors from the crystal structure (purple) and simulated average structures from the unit cell (green) and supercell (cyan) simulations. (B) Residue-wise RSCC computed between the crystal structure and the charge density from the supercell (green) and unit cell (cyan) simulations.