BIOCHEMISTRY
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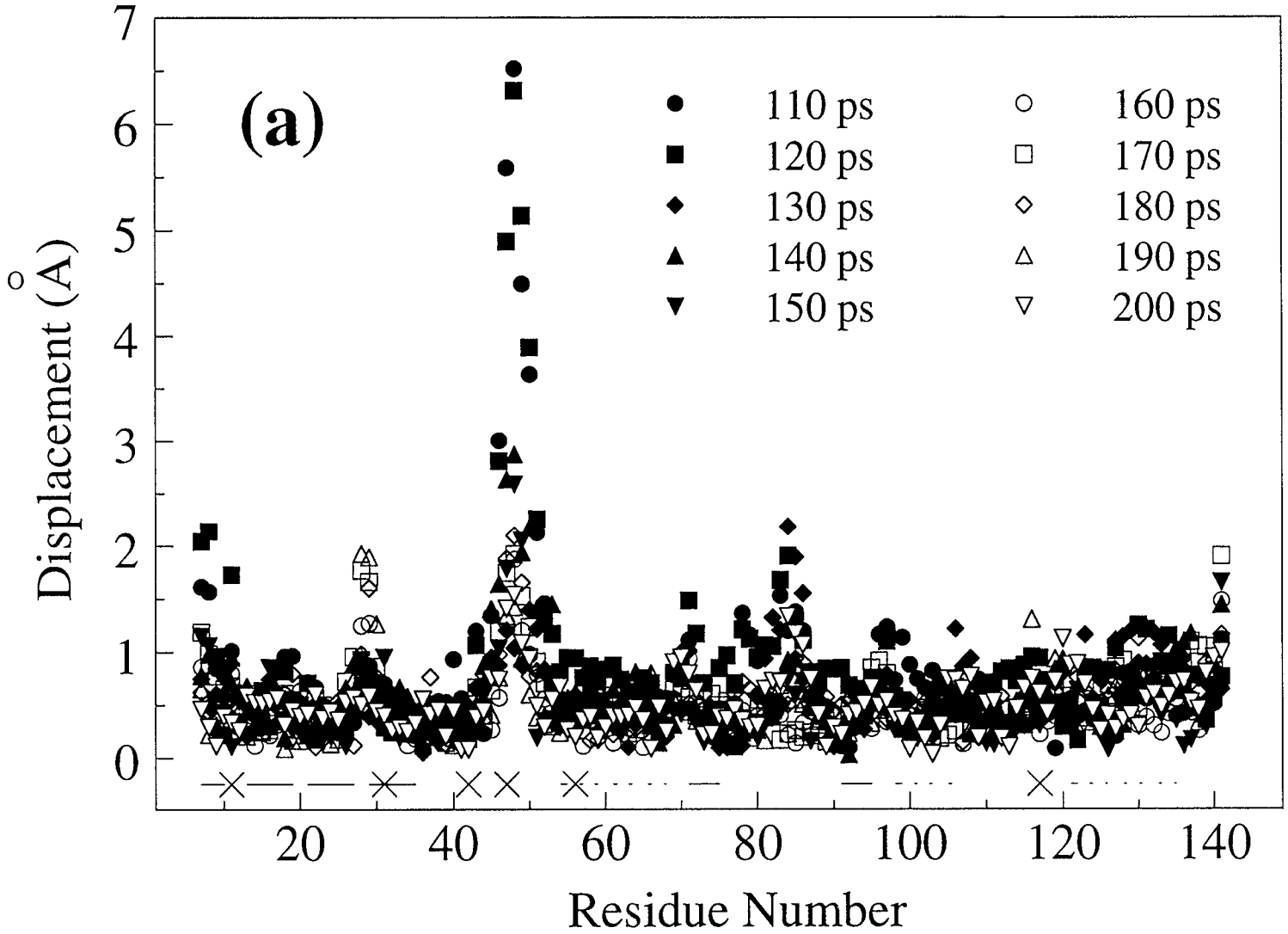
Supporting Information for Microfilm Edition

Figure S-1. Displacements between C^{α} atoms of the transient structures and the structure averaged over the structures observed during the molecular dynamics simulations of wild-type SNase in vacuo (a) and in water (b). (c) The *B* factors of C^{α} atoms of SNase in the monomeric structure without Ca^{2+} and pdTp (solid line) and in the ternary complex with Ca^{2+} and pdTp (dashed line) determined by the X-ray crystallographic studies (Hynes & Fox, 1991; Loll & Lattman, 1989). At the bottom of each panel, the continuous segments represent β-strands, the dotted segments α-helices, and the crosses Pro positions.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130 ps
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170 ps
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200 ps
Displacement (Å)
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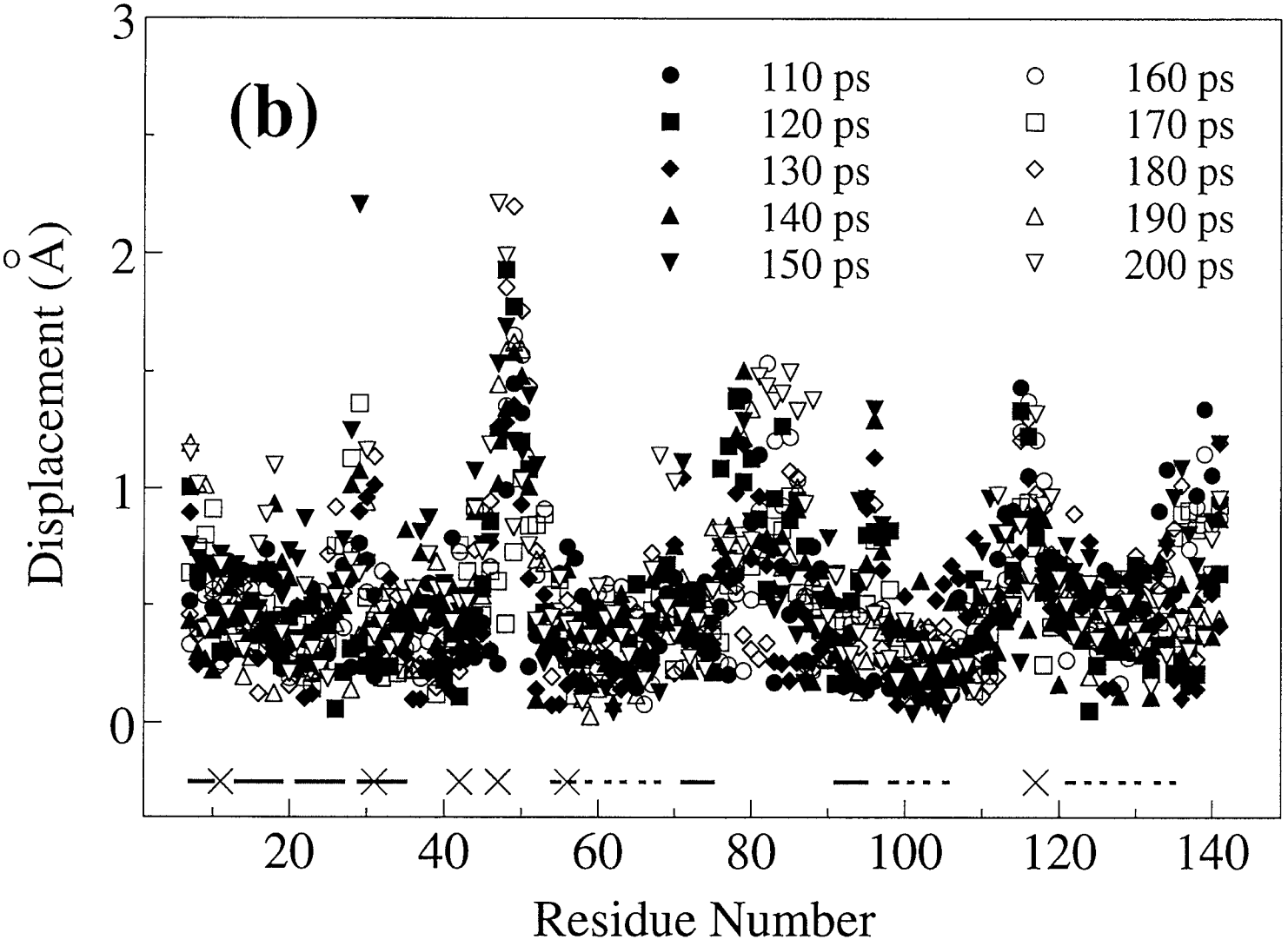
(b)
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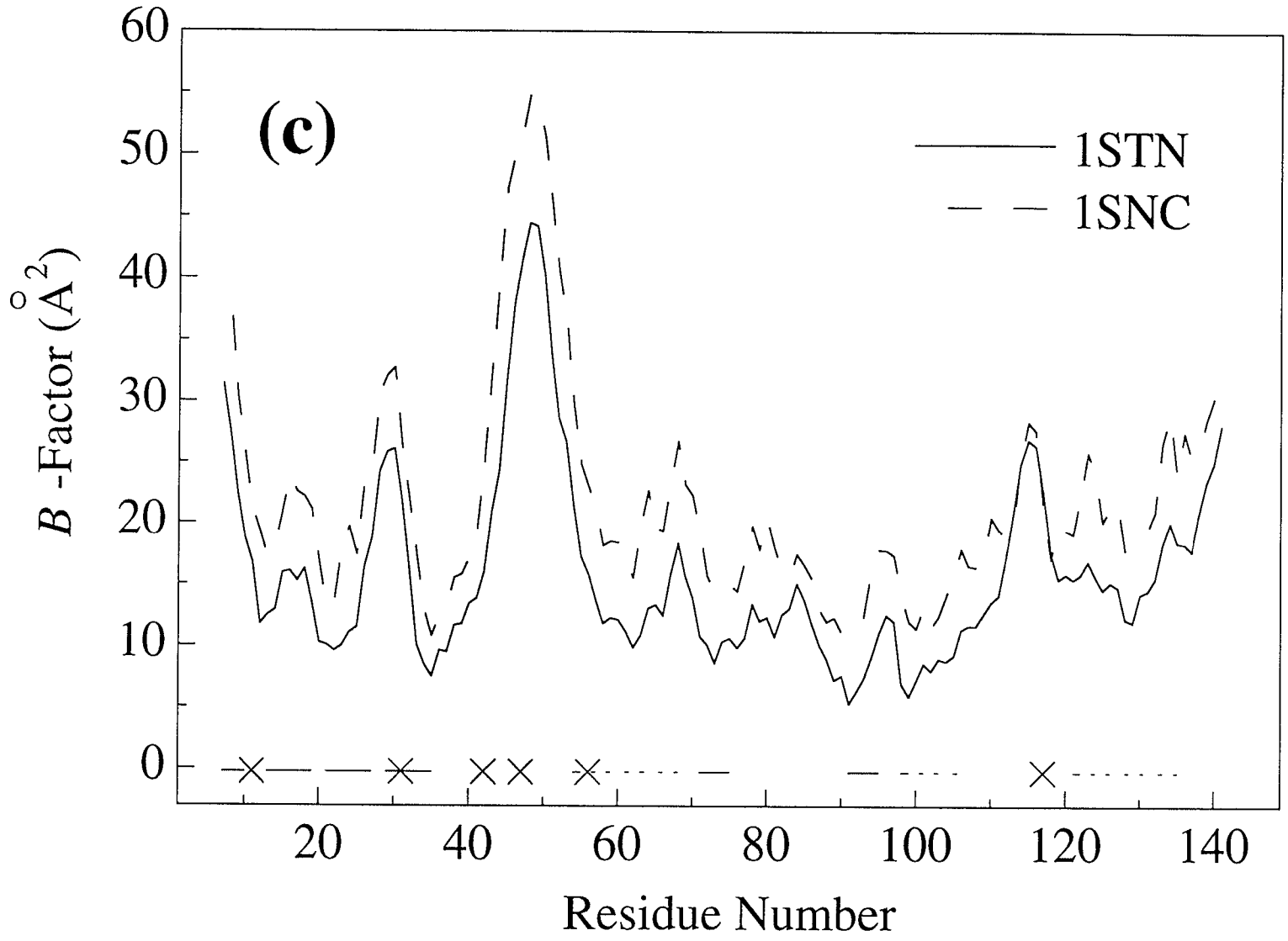
(c)
1STN
1SNC
B -Factor (Å²)
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100
120
140