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Supporting Material

Focused Functional Dynamics of Supramolecules by Use of a Mixed-Resolution Elastic Network Model

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Supplementary Figures:

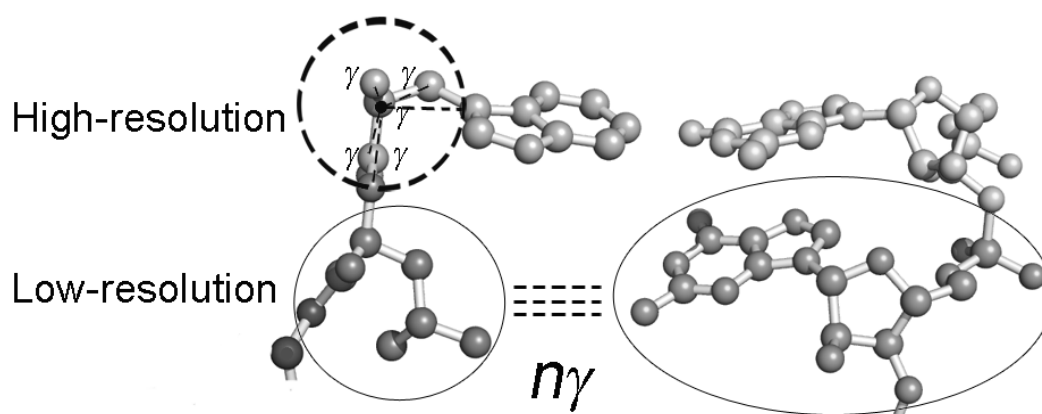


FIGURE S1. Determination of the interaction cutoff (dotted circle) and the interaction forces (dotted lines) using the new atom-based approach. All neighboring heavy atoms of both amino acids and nucleotides in the crystal structure are linked with a single spring (γ). In the high-resolution region, node pairs (heavy atoms) are linked with a single spring. In the low-resolution region (group of residues), the coarse-grained nodes (full circles) are linked with multiple springs that connect their multiple atom pairs of these coarse-grained nodes.

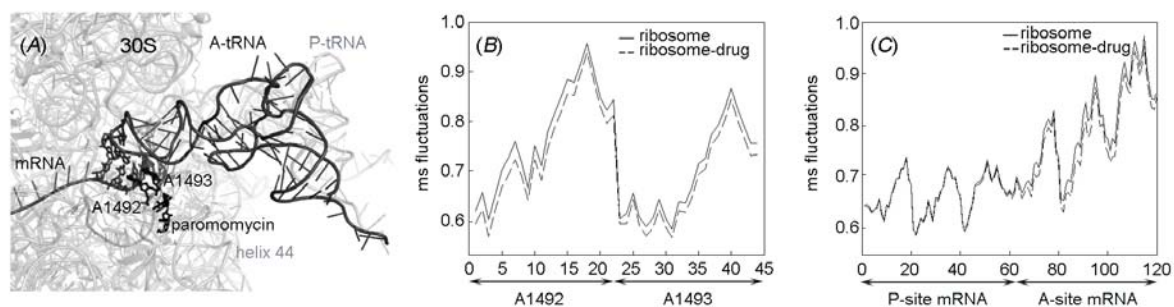


FIGURE S2. (A) The binding site of the antibiotic paromomycin on the small ribosomal subunit near the decoding center. The high-resolution region of the ribosome model is shown in stick form. The ms fluctuations are averaged over the 100 slowest modes for the ribosome, free (solid line) and drug bound (dotted line). The fluctuations are shown for (B) the decoding center and (C) the A- and P-sites of the mRNA.