

Structure 16

Supplemental Data

Multiple Conformations of *E. coli* Hsp90 in Solution: Insights into Conformational Dynamics of Hsp90

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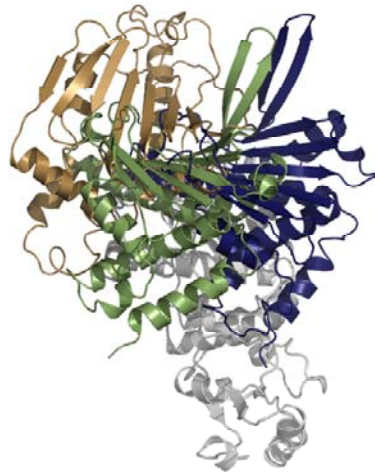


Figure S1. The Modeled NM Domain Represents a Structure Intermediate between the Apo Crystal Structure and the AMPPNP Bound Crystal Structure

The NM domains from the apo crystal structure (blue), the AMPPNP homology model (brown), and the best fitting NM domain model (green) aligned by their middle domains.

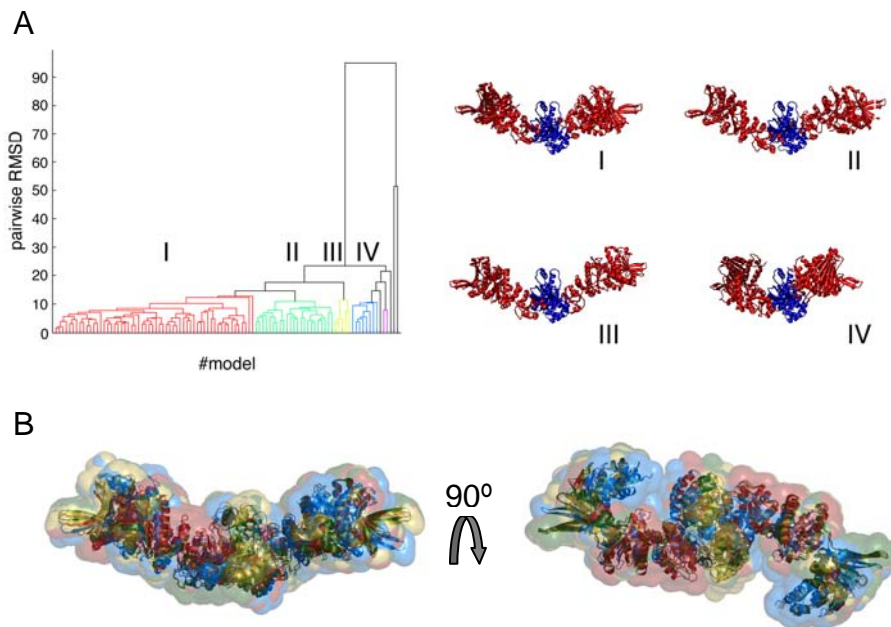


Figure S2. Clustering of the Models for the Full-Length Apo HtpG SAXS Data

A) Clustering of the top 10% of the best scoring models created for fitting the apo HtpG SAXS data. The structures represent the top scoring model from each cluster, respectively.

B) Two views of the alignment of the volumes of the four top models.

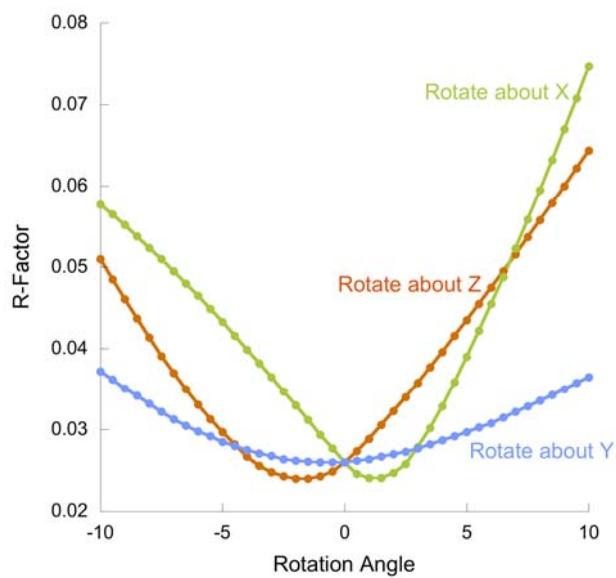


Figure S3. Effects of Small Motions on the Fit of the Model to the Full-Length Apo HtpG Scattering Data

Plot of the degree of rotation of the arms of the HtpG dimer versus the fit to the experimental data. The arms of the open model were rotated by small degrees in the direction of x, y, and z and the fit of the new model calculated from the distance distribution functions. The final optimum is well determined.

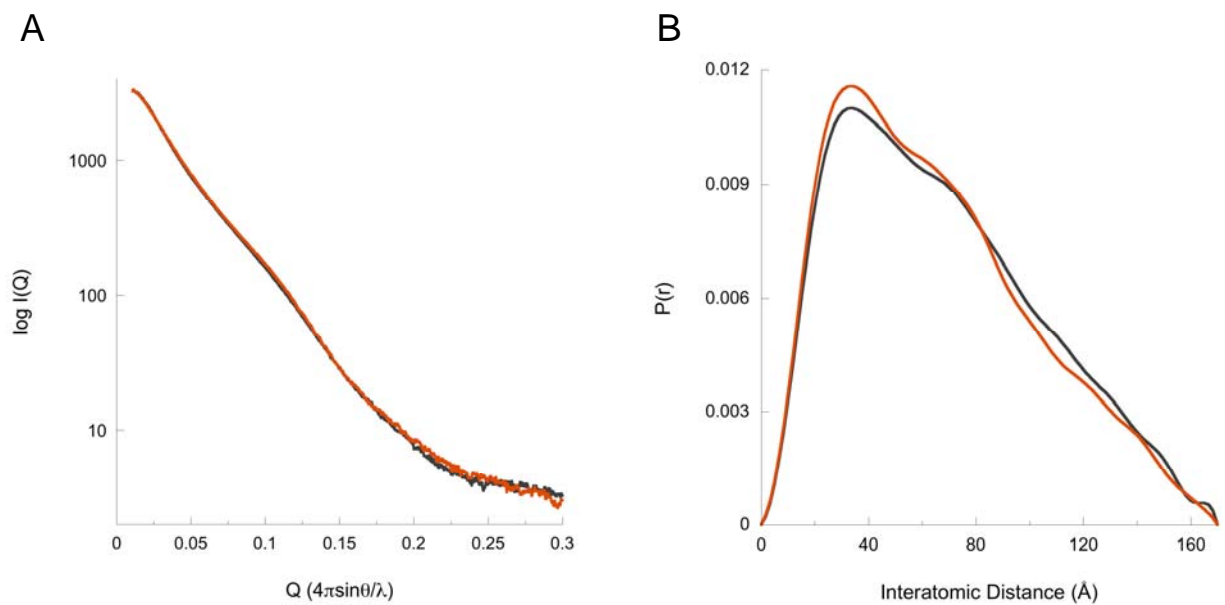


Figure S4. Comparing Apo and ADP-bound HtpG by SAXS

A) Averaged and scaled solvent-subtracted scattering curves ($I(Q)$) for full length HtpG in the absence of nucleotide (black) and in the presence of saturating amounts of ADP (10 mM ADP, red).

B) Interatomic distance distribution functions ($P(r)$) calculated from the scattering data shown in panel A (black and red for apo and ADP-HtpG, respectively). The $P(r)$ curves are normalized to have equivalent areas under the curve.