Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Design of a structure-based model for protein folding from flexible conformations

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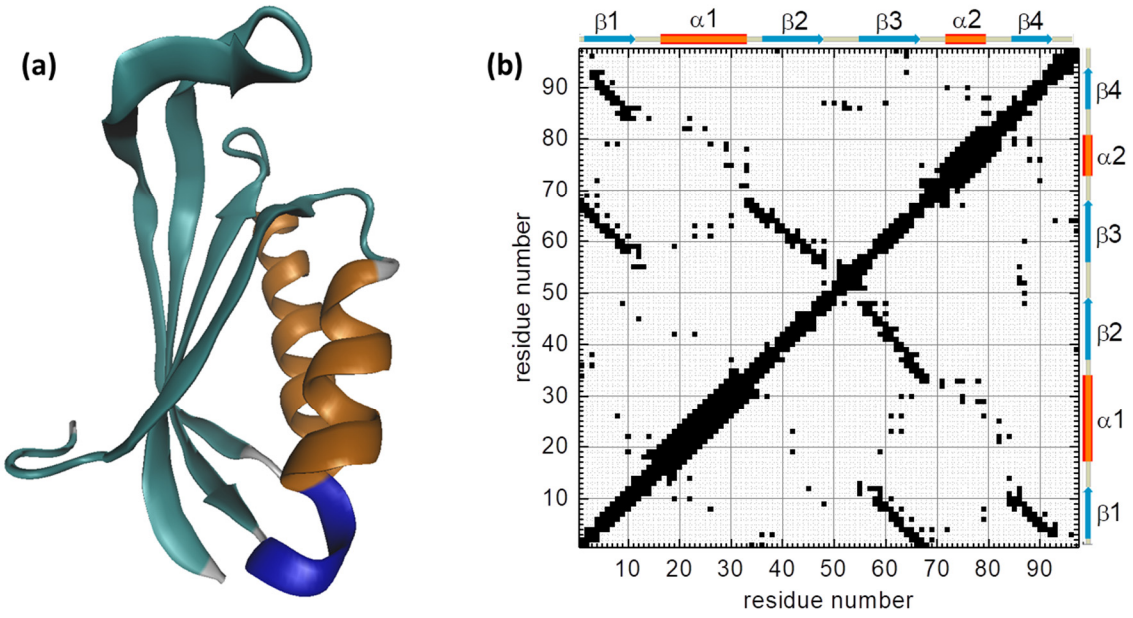
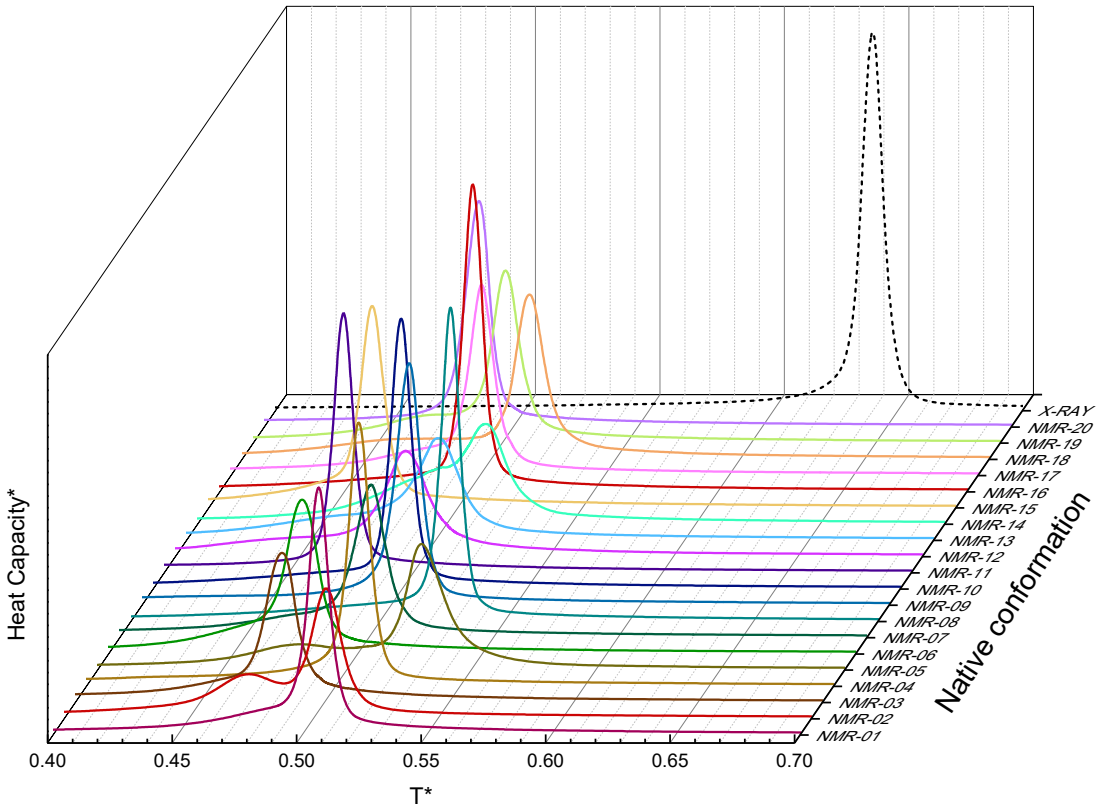
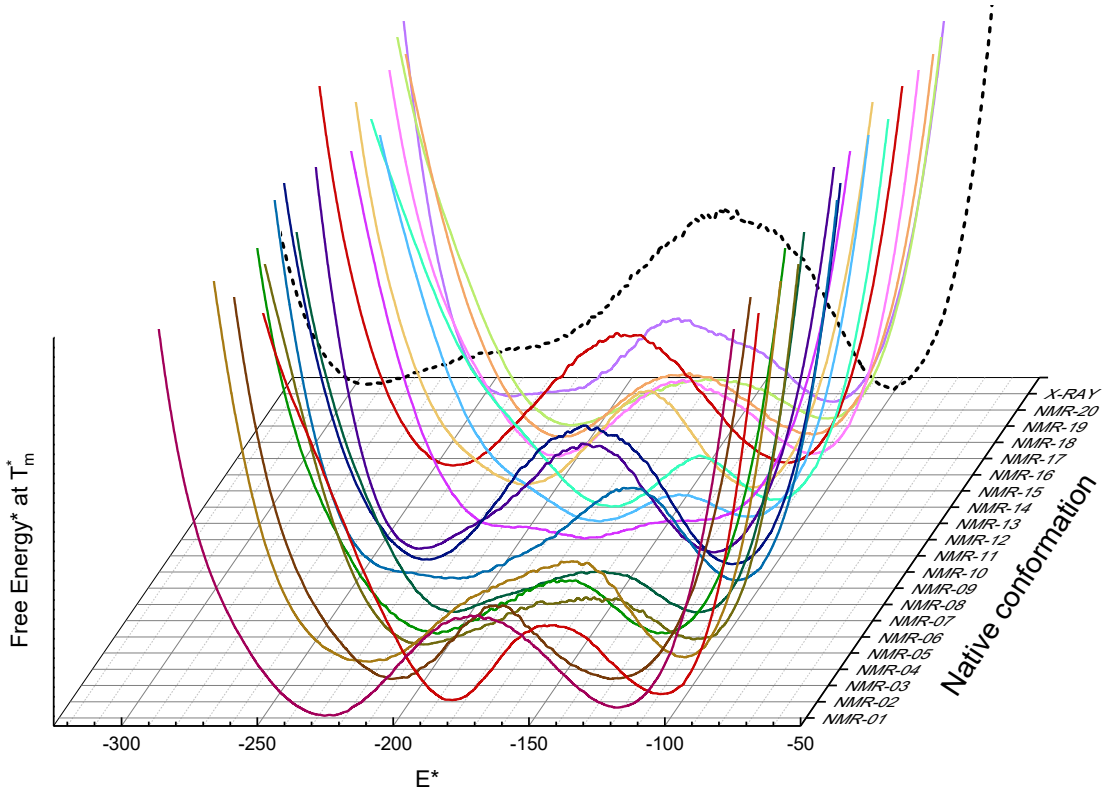
ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)



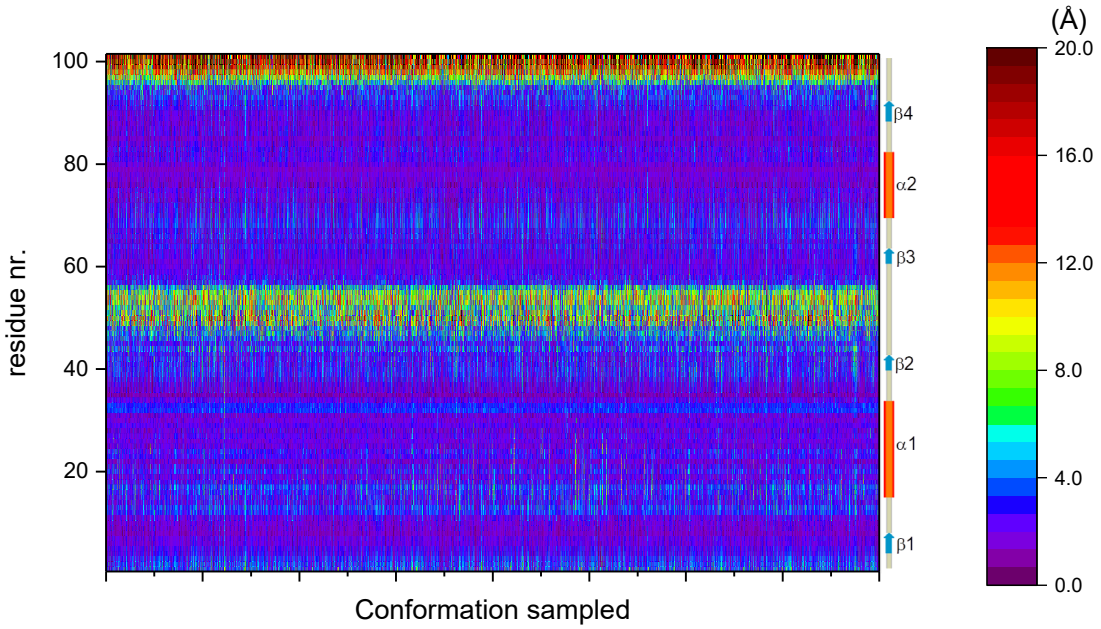
Supplementary Figure S1. Ribbon diagram and contact map for the x-ray structure of protein S6, as taken from the PDB file 1RIS. The positions of the secondary structure elements along the sequence are sketched at the axes of the contact map.



Supplementary Figure S2. Heat capacity curves (in reduced units) as a function of the reduced temperature, from standard structure-based calculations (based on a single structure, as indicated in the right axis).



Supplementary Figure S3. Free energy curves (in reduced units) as a function of reduced energy, from standard structure-based calculations (based on a single structure, as indicated in the right axis). The native basin appears at the left side (lower energy).



Supplementary Figure S4. Plot of the structural fluctuations after optimal superposition for a representative set of 8000 conformations along the simulation for T = 0.9 T_m in the NMR-Global model. The NMR-01 conformer from the PDB file 2KJV is used as reference structure.