

SUPPLEMENTARY INFORMATION

Structural Characterization of Flexible Proteins Using Small-Angle X-ray Scattering

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FIGURE S1.

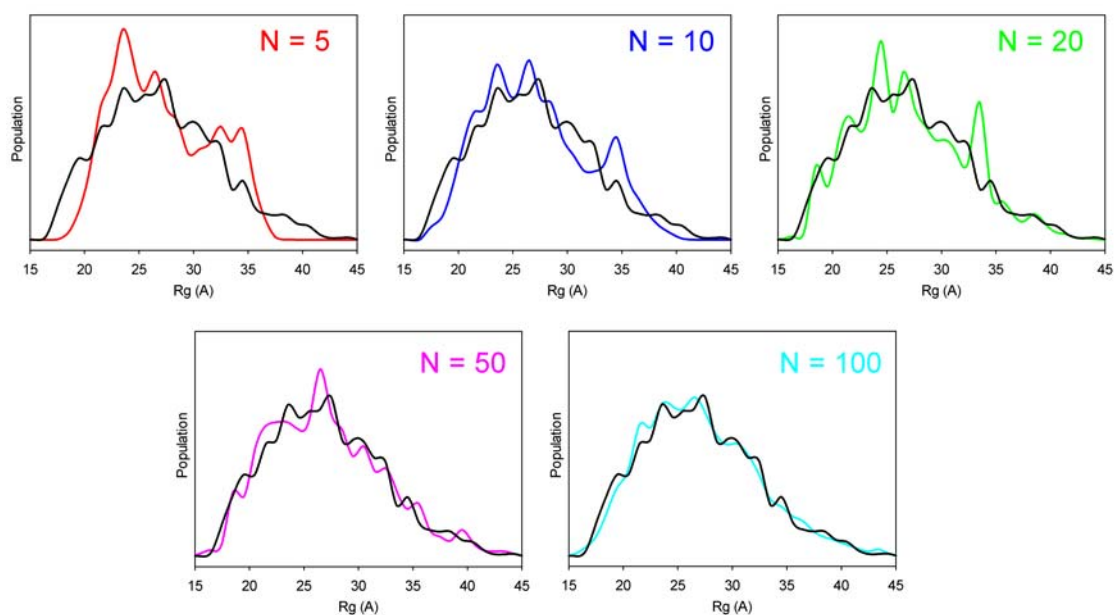


Figure S1. Effect of the size of the chromosomes on the performance of the EOM for the polyaniline free chain test-case (*control*). R_g distribution for chromosomes with N values of 5 (red), 10 (blue), 20 (green), 50 (pink) and 100 (cyan), compared with the one derived from a 1,000 structures of the polyaniline chain without restrictions, *control* , (black).

FIGURE S2.

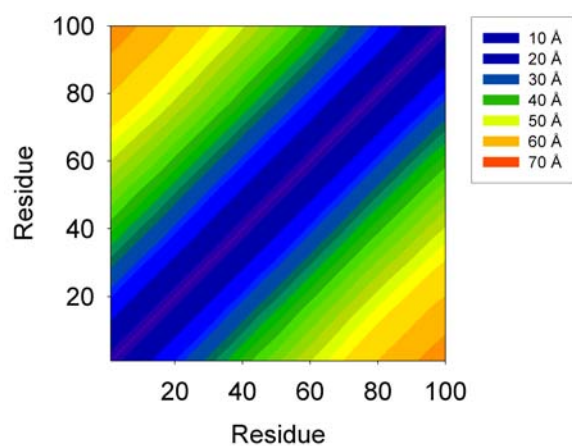


Figure S2. Average $C_\alpha - C_\alpha$ distance matrix for the pool of 10,000 structures of the polyaniline chain. The color scale goes from less than 10 Å (purple) to 70 Å in red.

FIGURE S3

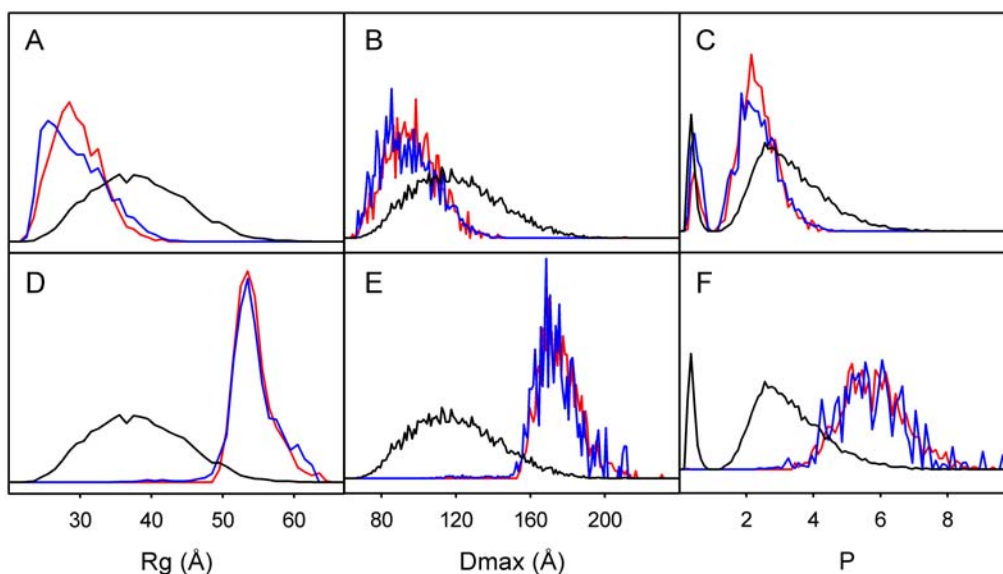


Figure S3. Size and shape descriptor distributions obtained from the analysis of the optimized ensemble of scattering profiles calculated for polyubiquitin chains with restricted conformational sampling. (A-C) polyubiquitin chain with a contact (< 30 Å) between the centers of mass of the first and the third ubiquitin domains of the chain (*symmetric compact*). (D-F) restricted polyubiquitin chain forcing the centers of mass of the first and the fourth ubiquitin domains to be separated by more than 130 Å (*symmetric extended*). Distributions from the pool, the simulated and the fitted ensembles are shown in black, red and blue, respectively.

FIGURE S4

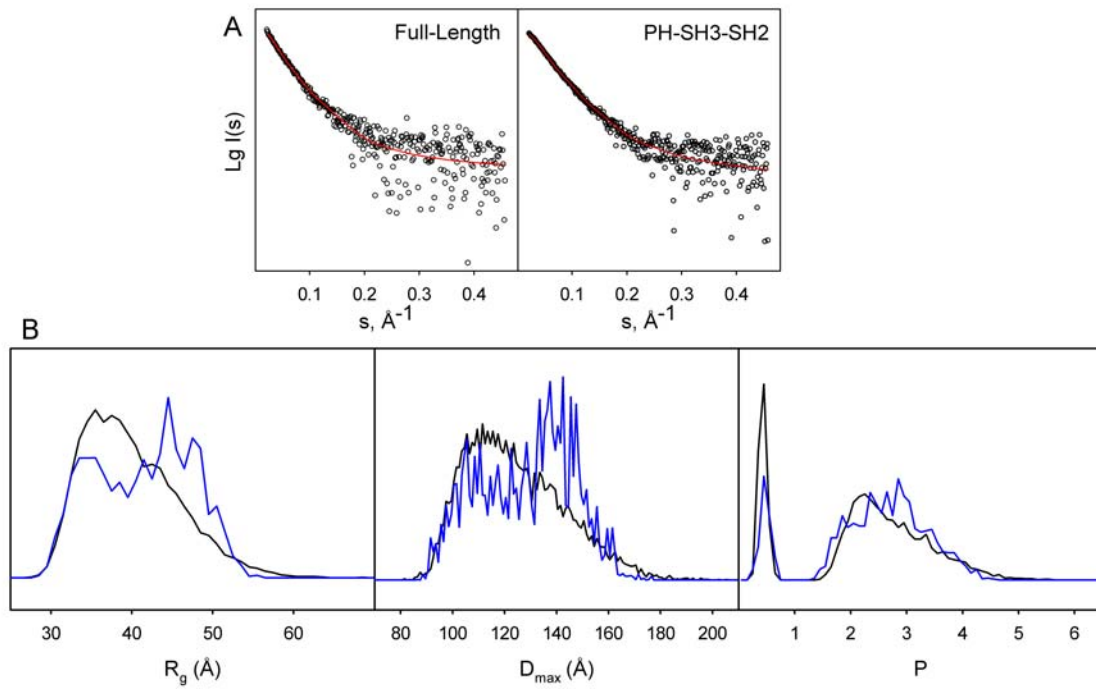


Figure S4. Application of the EOM to BTK. (A) Experimental data (black) and the multiple curve fitting (red) performed with the EOM for both used constructs. (B) Size and shape descriptor distributions (R_g , D_{max} , and P) derived from the ensemble of structures the simultaneously fitted the BTK scattering profiles (Full-Length and PH-SH3-SH2 constructs; black: pool, blue: EOM subset).