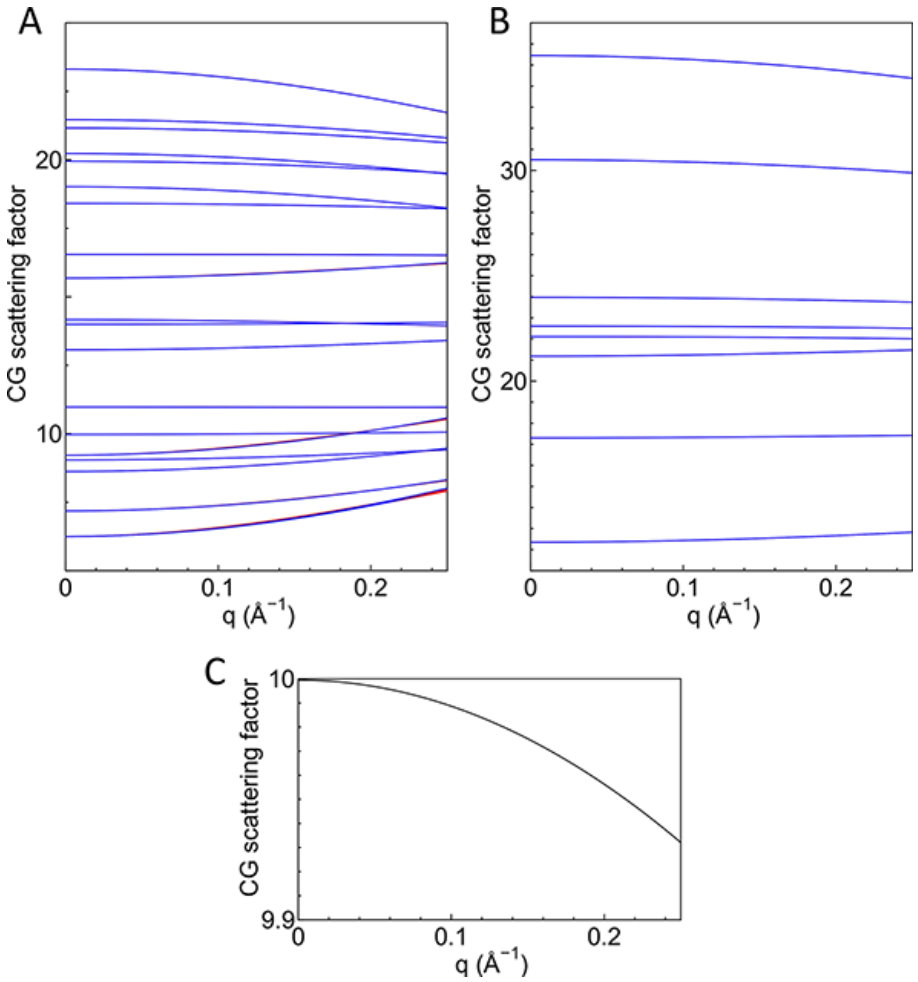
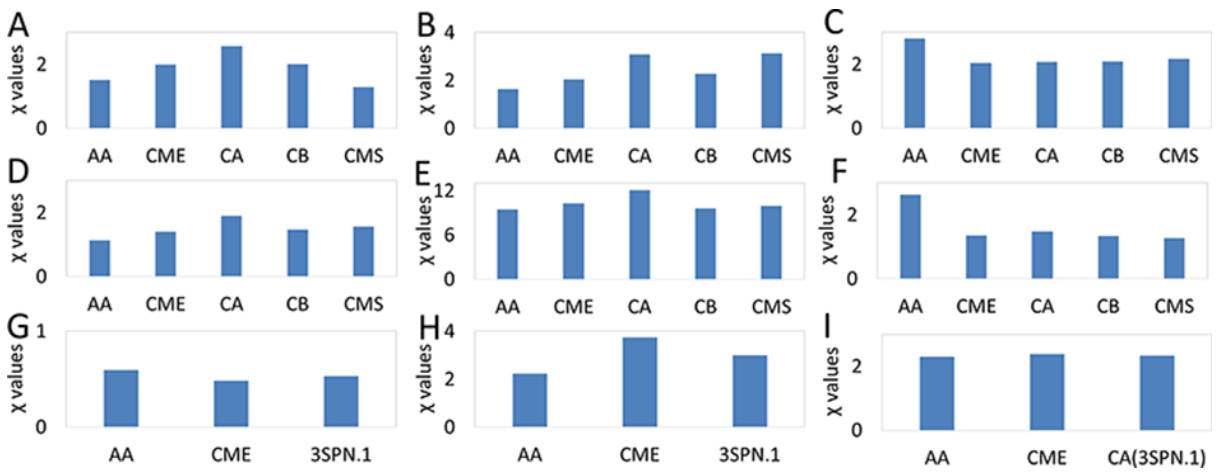


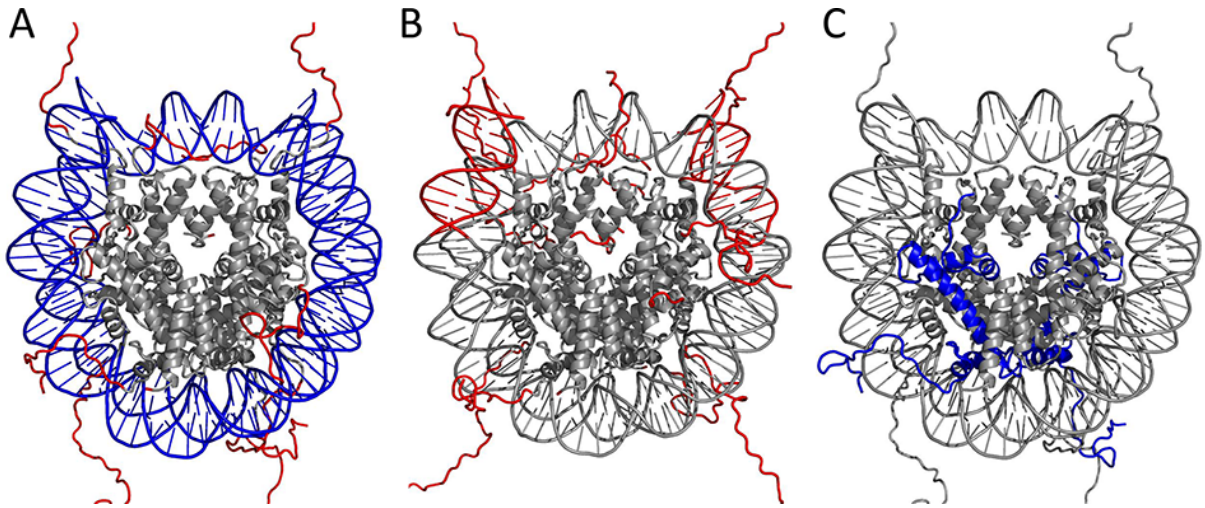
Supplementary Figure S1. CG scattering factors for amino acids and nucleic acids, and the scattering intensity of a water molecule.

(A) The CG scattering factors for ARG, HIS, ASP, GLU, ASN, GLN, CYS, MET, TRP, TYR, SER, THR, LYS, GLY, PHE, ALA, PRO, VAL, LEU, and ILE from top to bottom at q = 0. The scattering factors including excluded-volume effects derived from Eqs. (7) and (8) are represented as red and blue lines, respectively. (B) The atomic scattering factors of nucleic acid for guanine, adenine, phosphoric acid, cytosine, uracil, thymine, ribose, and deoxyribose from top to bottom at q = 0. (C) The scattering intensity of a water molecule.

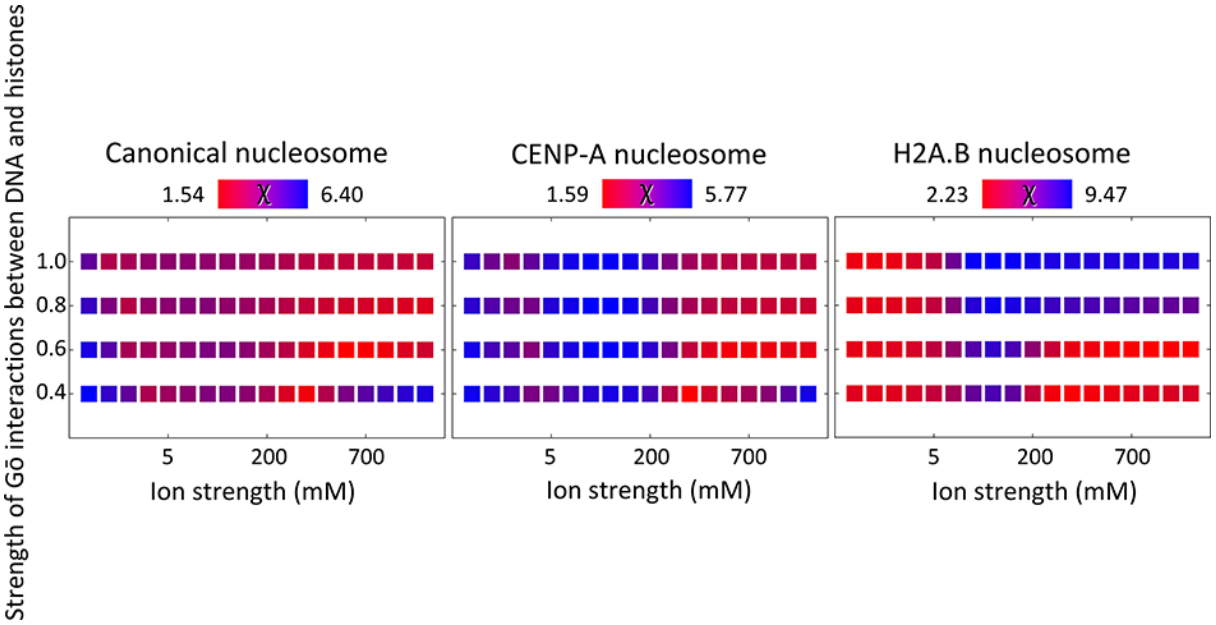


Supplementary Figure S2. The χ values obtained using the various CG models and the all-atom model.

The examined CG models for protein were as follows: the center of electrons (CME model), Cα position (CA model), Cβ position (CB model), and the center of the side chain of each residue (CMS model). For nucleic acids, the CME model and the 3SPN.1 model were examined. The χ value obtained using the all-atom model is represented by AA. The theoretical SAXS profiles for the all-atom models were calculated using CRYSOL. (A) Immunoglobulin-like domains 1 and 2 of the protein tyrosine phosphatase LAR3 (BIOISIS ID: LAR12P). (B) Superoxide dismutase (BIOISIS ID: APSOD). (C) Ubiquitin-like modifier-activating enzyme ATG7 C-terminal domain (BIOISIS ID: ATG7CP). (D) DNA double-strand break repair protein MRE11 (BIOISIS ID: MRERAP). (E) Glucose isomerase (BIOISIS ID: GISRUP). (F) Complement C3b + Efb-C (BIOISIS ID: C3BEFP). (G) 28 base-pair DNA (BIOISIS ID: 28BPDD). (H) The P4-P6 RNA Ribozyme domain (BIOISIS ID: 1P4P6R). (I) *A. aeolicus* MnmG bound to tRNA (BIOISIS ID: MNMG2X).



Supplementary Figure S3. Model structures of the nucleosomes.
(A) The canonical nucleosome. Added histone tails are shown in red. DNA sequences colored blue were changed. (B) The CENP-A nucleosome. Added histone tails and DNA are shown in red. (C) The H2A.B nucleosome. H2A.B is shown in blue.



Supplementary Figure S4. χ values obtained using the CG-MD-SAXS method.
CG-MD simulations for three nucleosomes were performed by changing two parameters: the ion strength and the strength of Gō interactions between DNA and histones. Squares represent CG-MD simulations under various conditions, and the colors in squares indicate the χ values calculated using the CG-MD-SAXS method. The minimum and maximum values of χ values are shown in the color bar.