

Analyzing Bending Energy in the Nuclear Pore Complex from a Point Cloud Representation

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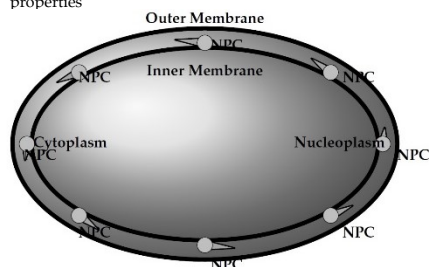
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ABSTRACT

The **Nup54/Nup58 complex**, a critical component of the Nuclear Pore Complex (NPC), regulates the flexibility and diameter of the NPC's transport channel, adapting to varying cargo sizes. Using structural data from PDB entry **3T98**, which represents a segment of the Nup54/Nup58 ring, we analyze its bending energy and flexibility through computational modeling.

Applying the **Helfrich model** in a discrete form, we compute the bending energy by deriving curvatures and surface area elements from the point cloud representation of 3T98. Our analysis of this dynamic NPC component provides insights into the energetic properties



Nuclear Envelope with Nuclear Pore Complexes (NPCs)

Figure 1. Schematic representation of the nuclear envelope showing the inner and outer membranes and nuclear pore complexes (NPCs).

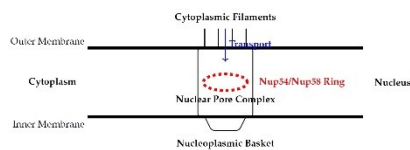


Figure 2. Schematic representation of the nuclear pore complex (NPC), highlighting key structural components such as the Nup54/Nup58 ring, cytoplasmic filaments, and nucleoplasmic basket

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METHODOLOGY FOR DATA PROCESSING

Dataset Acquisition:

Structural data for the Nup54/Nup58 complex was obtained from PDB entry 3T98.

This dataset represents a segment of the Nup54/Nup58 ring, capturing interacting domains between these nucleoporins.

Surface Representation:

The .cif file was processed in Chimera, where the molecular surface was visualized using the hydrophobic surface preset and the protein preset.

The structure was exported as a .obj file, capturing the molecular surface geometry.

Point Cloud Generation:

The .obj file was imported into MeshLab, which exported the structure as a .xyz file (point cloud format containing coordinates and normals).

Point Cloud Preparation:

The .xyz file was loaded into CloudCompare, where the data was further refined and converted into the .pcd format (Point Cloud Data) for computational analysis.

METHODOLOGY FOR COMPUTATIONAL AND PHYSICAL ANALYSIS

Curvature and Area Computation:

Using the Point Cloud Library (PCL), the following properties were computed for each point in the cloud:

Mean curvature (H): Average surface bending. Gaussian curvature (K): intrinsic curvature based on the product of the principal curvatures.

Area elements (ΔA): Local surface area around each point.

Bending Energy Calculation:

The bending energy was estimated using the Helfrich model in its discrete form:

$$E = \sum_{i=1}^N [k/2 (2H_i - C_0)^2 + k_c K_i] \Delta A_i$$

Algorithmic application:

Algorithms are applied on the Point Cloud dataset to compute curvatures (H and K), local surface area elements (ΔA). Filtering the area elements (ΔA) and finally computing the bending energy.

RESULTS

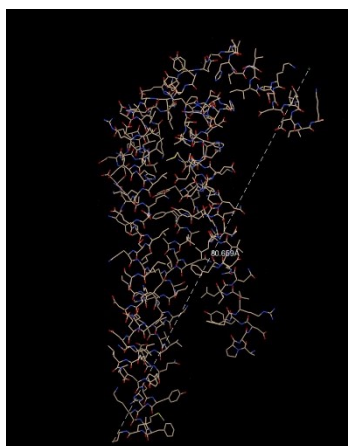


Figure 3. The Nup54/Nup58 structure open in Chimera using a protein display where the diagonal distance was measured to be about 80,659 Å or about 8.0659 nm

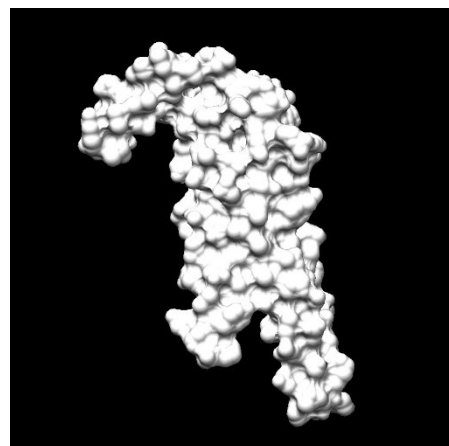


Figure 4. The Nup54/Nup58 structure open in Meshlab showing the hydrophobicity surface geometry

COMPUTATIONAL RESULTS

The calculated bending energy of 1.15363×10^{20} J aligned with the expected range for flexible protein structure. This suggests that the Nup54/Nup58 ring segment exhibits a degree of flexibility comparable to other biomolecule complexes.

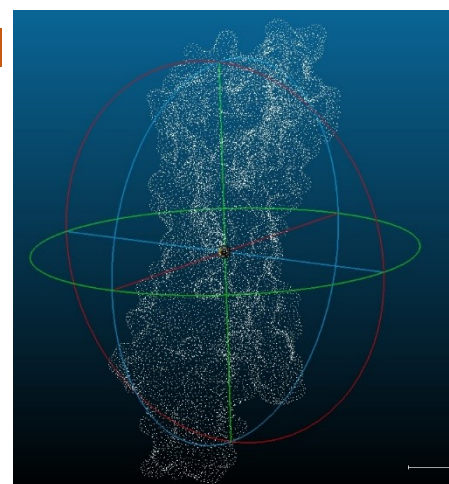


Figure 5. The Nup54/Nup58 structure open in CloudCompare, displayed in point clouds, showing the dataset ready for further computational analysis