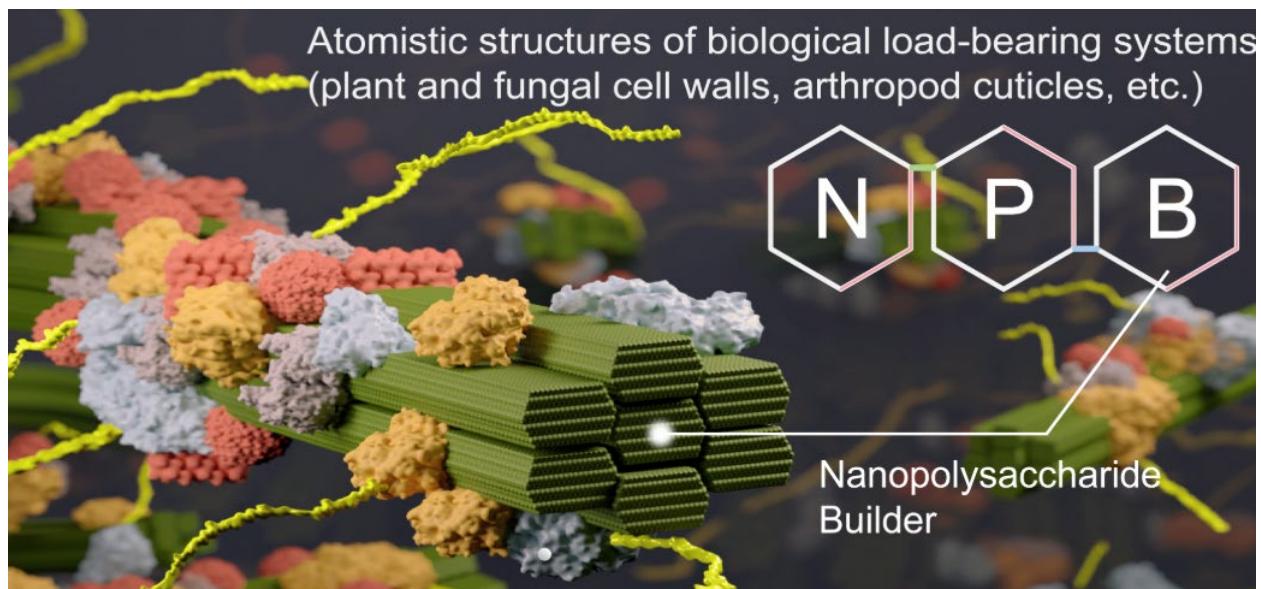


Nanopolysaccharide Builder (NPB)

A User-Friendly Tool for Atomistic Models of Polysaccharide-Based Nanostructures



USER MANUAL

Nanopolysaccharide Builder: A User-Friendly Tool for Atomistic Models of Polysaccharide-Based Nanostructures

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This NPB user manual provides guidance on using the software package to prepare structures and topology files required for simulations of cellulose, chitin, and their bundle nanostructures. It supports both **CHARMM36** and **GLYCAM06j** force fields for nanopolysaccharides. This tutorial offers step-by-step instructions for preparing all necessary files for simulations in **NAMD**, **AMBER**, and **GROMACS**.

Disclaimer

The programs and scripts in the NPB package are provided without any guarantees or warranties, either explicit or implied. The authors are not responsible for any issues or damages that may arise from using this software. The NPB tool and manual will be updated as new features become available, so users are encouraged to use the latest version. For questions, comments, or problems, please submit an issue in the NPB public repository:

<https://github.com/Hugo-Wan/Nanopolysaccharide-Builder>

Citing NPB

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1. NPB Package Installation

The dependencies can be installed using one of the following methods on a Unix-like system (e.g., Ubuntu 24.04). A brief introduction to installing NPB on macOS is also provided in **Chapter 1.3**.

1.1 Installation of Ubuntu

Linux users can skip this step. This section is intended specifically for Windows users running a virtual machine. You can use either WSL or VMware to install a Linux system; here, we demonstrate the process using VMWare.

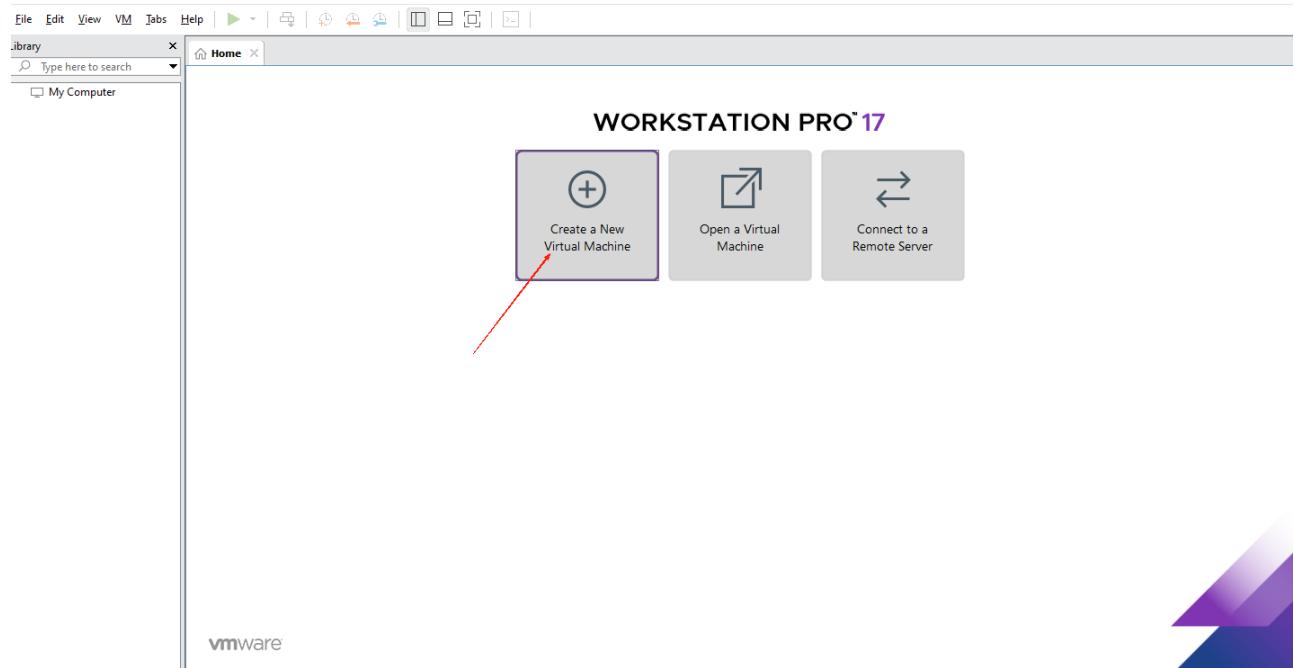
User can download VMWare from here:

<https://www.vmware.com/products/desktop-hypervisor/workstation-and-fusion>

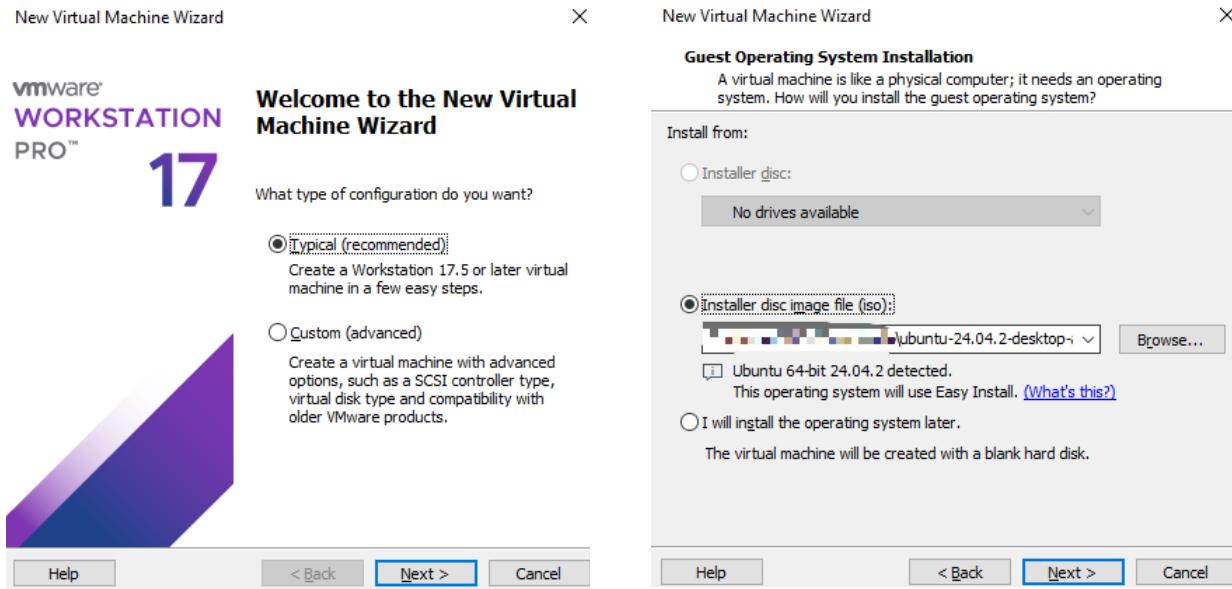
Ubuntu-24.04 form here:

<https://ubuntu.com/download/desktop>

Step 1. Create a New Virtual Machine

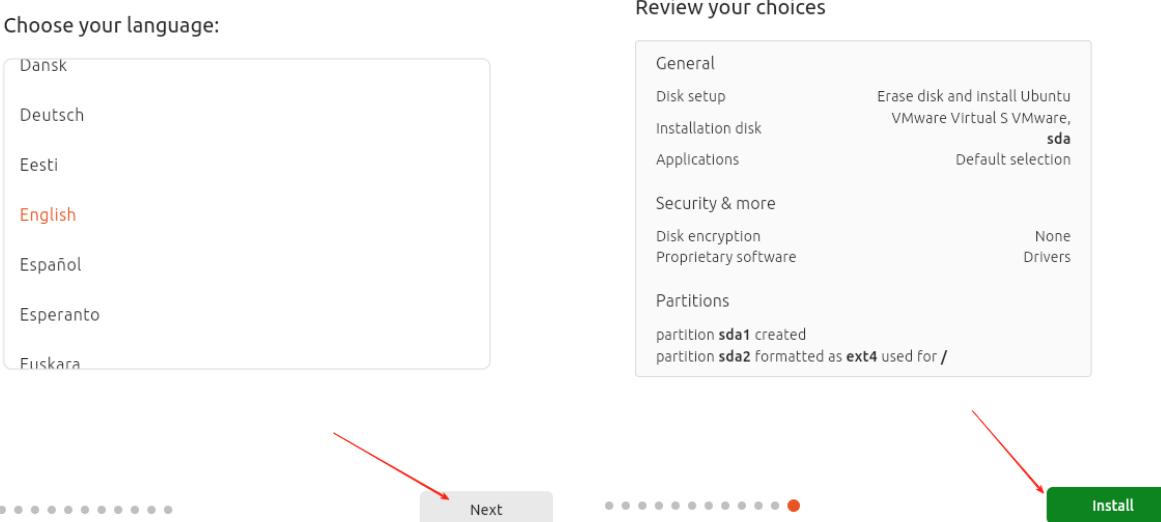


Step 2. Click **Typical** installation, selection of the **Ubuntu ISO file**, and followed by clicking



Next

Step 3. Always click **Next** when prompted, fill in the required information, and then click the **Install** button to continue.



If the user encounters any issues during the Ubuntu installation, they can use this video for more detailed steps:

https://www.youtube.com/watch?v=SgfrHKg81Qc&ab_channel=ProgrammingKnowledge

1.2. Installation of NPB

Step 1. For a new system, users can install the necessary system dependencies by entering the provided commands in the terminal (opened with Ctrl+Alt+T). If the user already has a Linux system set up, this step can be skipped. Type the following script in the terminal.

```
1 | sudo apt-get install build-essential
```

Step 2. Installing python environment (miniconda recommended). User can download miniconda from the website:

<https://www.anaconda.com/docs/getting-started/miniconda/install#linux-terminal-installer>

Getting Started > Miniconda

Installing Miniconda

Using Miniconda in a commercial setting?

This page contains basic Miniconda installation instructions for Windows, macOS, and Linux, as well as a command-line quickstart installation guide.

ⓘ On Windows, macOS, and Linux, it is best to install Miniconda for the local user, which does not require administrator permissions and is the most robust type of installation. However, if you need to, you can install Miniconda system wide, which does require administrator permissions.

Basic install instructions

Windows installation

macOS/Linux installation

macOS graphical installer macOS terminal installer Linux terminal installer

1. Download the latest version of Miniconda by opening a terminal and running one of the following commands (depending on your Linux architecture):

Linux x86 AWS Graviton2/ARM64 IBMZ/LinuxOne/s390x

Here, users can select the Linux x86 version. If using a different Linux platform, choose the appropriate version of Miniconda. Typing the following scripts in the terminal (opened with Ctrl+Alt+T)

```
1 wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
2
3 bash ~/Miniconda3-latest-Linux-x86_64.sh
4
5 source ~/.bashrc
```

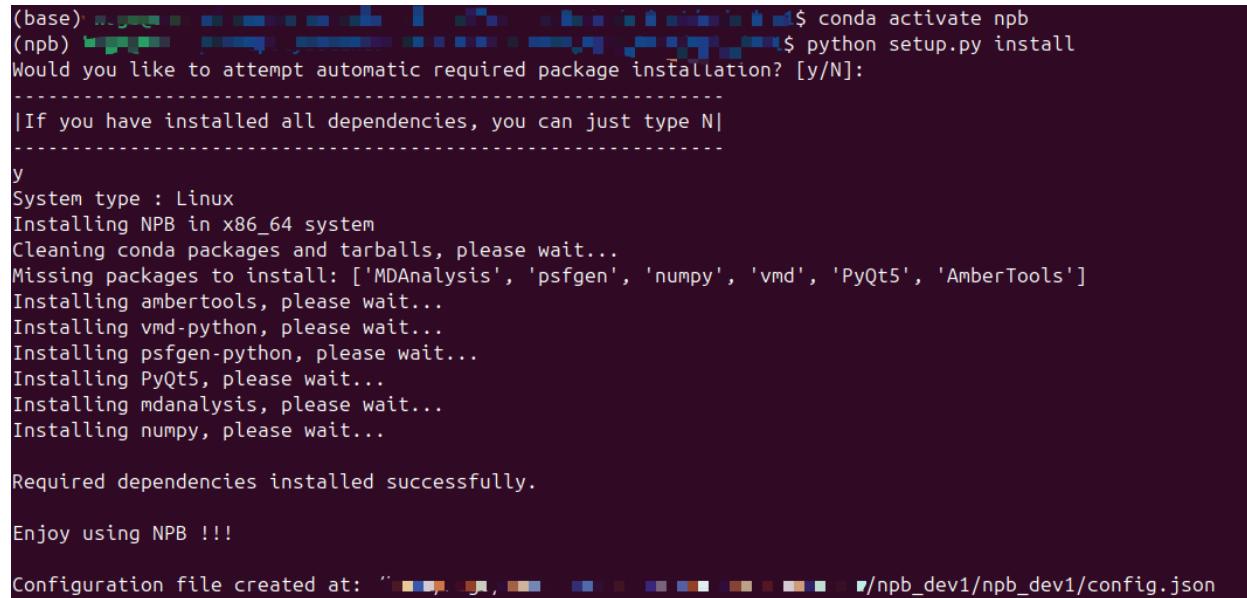
Step 3. Building a Python virtual environment (a clean environment is recommended): Users can type the following scripts in the terminal (opened with Ctrl+Alt+T) to create a fresh environment for installing the NPB package. Unzip the compressed file and navigate to the NPB package folder to install the required dependencies. Type the following scripts in the terminal (opened with Ctrl+Alt+T). (Remember to unzip the compressed file).

```

01 # (Optional) Create a new environment named "npb" with Python 3.10 and requests
02 conda create -n npb python=3.10 requests
03
04 # Activate the environment
05 conda activate npb
06
07 # Navigate to the npb_dev1 folder
08 cd npb_dev1
09
10 # Install the package
11 python setup.py install
12
13 # After installation, start the GUI with:
14 python gui.py

```

After completing these steps, users can begin using the NPB package. A snapshot of a successful installation is shown in Figure 1. We have also tested the installation on Darwin systems (macOS x86 and macOS ARM), and both are compatible. However, because macOS differs from Linux, installation of certain dependencies, such as **psfgen-python** and **vmd-python**, may fail. Therefore, we recommend using a Linux system for installation to minimize the risk of errors.



```

(base) [REDACTED] $ conda activate npb
(npb) [REDACTED] $ python setup.py install
Would you like to attempt automatic required package installation? [y/N]:
-----|If you have installed all dependencies, you can just type N|
-----
y
System type : Linux
Installing NPB in x86_64 system
Cleaning conda packages and tarballs, please wait...
Missing packages to install: ['MDAnalysis', 'psfgen', 'numpy', 'vmd', 'PyQt5', 'AmberTools']
Installing amberTools, please wait...
Installing vmd-python, please wait...
Installing psfgen-python, please wait...
Installing PyQt5, please wait...
Installing mdanalysis, please wait...
Installing numpy, please wait...

Required dependencies installed successfully.

Enjoy using NPB !!!

Configuration file created at: [REDACTED] /npb_dev1/npb_dev1/config.json

```

Figure 1. Snapshot of a successful installation step in a virtual machine (Ubuntu 24.04).

1.3. Installation of NPB on macOS

If users are not familiar with Linux systems or have a Mac computer without sufficient disk space to install a virtual machine, we provide steps for installing NPB directly on macOS. Installation has been tested on both macOS-x86 and macOS-ARM architectures, including M1, M2, and M3 chips. All dependencies were successfully installed on M1 and M3 systems; however, installation on M2 failed due to issues with python-psfgen in the Miniconda environment. Below, we outline the general installation procedure for macOS-x86 systems.

Note: When installing Miniconda, be sure to choose the version that matches your CPU architecture, as selecting the wrong version may cause installation failures. Additionally, before running the install script, make sure your conda installation is up to date. If you are unsure, you can check and update conda by entering the following command in the terminal:

```
01 # Update conda to the latest version
02 conda update -n base -c defaults conda
03
04 # (Optional) Create a new environment named "npb" with Python 3.10 and requests
05 conda create -n npb python=3.10 requests
06
07 # Activate the environment
08 conda activate npb
09
10 # Navigate to the npb_dev1 folder
11 cd npb_dev1
12
13 # Install the package
14 python setup.py install
15
16 # After installation, start the GUI with:
17 python gui.py
```

During the installation process, a poor network connection to the Conda servers may cause delays or interruptions in installing dependencies, potentially disrupting the automatic installation (see Figure 2). If this occurs, users can simply re-enter the “**python setup.py install**” command to restart the installation.

```
System type : Darwin
Installing NPB in Darwin (mac-osx-arm) system
Cleaning conda packages and tarballs, please wait...
Missing packages to install: ['MDAnalysis', 'psfgen', 'numpy', 'vmd', 'PyQt5', 'AmberTools']
Installing amber tools, please wait...
Installing mdanalysis, please wait...

Failed to install all the required dependencies:
STDOUT:
STDERR:
```

Figure 2. Snapshot showing a poor connection to the conda server disrupting installation process.

After completing these steps, users can begin using the NPB package. A snapshot of a successful installation in macOS-x86 is shown in Figure 3.



```
(base) npb_dev1 % conda activate npb
(npb) npb_dev1 % python setup.py install
Would you like to attempt automatic required package installation? [y/N]:
|If you have installed all dependencies, you can just type N|
y
System type : Darwin
Installing NPB in Darwin (mac-osx) system
Cleaning conda packages and tarballs, please wait...
Missing packages to install: ['MDAnalysis', 'psfgen', 'numpy', 'vmd', 'PyQt5', 'AmberTools']
Installing amberTools, please wait...
Installing mdanalysis, please wait...
Installing numpy, please wait...
Installing PyQt5, please wait...
Installing vmd-python, please wait...
Installing psfgen, please wait...

Required dependencies installed successfully.

Enjoy using NPB !!!
Configuration file created at: /npb_dev1/config.json
```

Figure 3. Snapshot of a successful installation step in a macOS-x86 system.

Notes: When installing NPB on a macOS ARM system, users may encounter issues with the installation of psfgen and vmd-python. If the automatic installation fails, try installing these dependencies manually. If psfgen-python remains incompatible with your ARM-based Mac, we recommend using a Linux environment via a virtual machine, as described in Chapters 1.1 and 1.2.

2. Construction of Cellulose Nanostructures

2.1. Native Cellulose

Studies on plant cellulose synthesis indicate that wood nanofibrils may contain as few as 36, 24, or even 18 cellulose chains (β -1,4-polyglucans). In addition to higher plants, pure cellulose I β is found in certain animal species, such as tunicates, while pure cellulose I α is present in the cell walls of some freshwater algae. For 18, 24, 36 chain model, NPB provides a hexagonal cross-section. For tunicate cellulose, users can select a parallelogram-shaped cross-section (1), and for algal cellulose, a rectangular (squarish) cross-section is available. Here three examples for building different cross-section shape of native cellulose.

2.1.a. Hexagonal Shape

Step 1. Select the “Cellulose Models” and “Cellulose-I Builder” buttons, then use the drop-down menu to choose either **Cellulose-I β** or **Cellulose-I α** . Next, select your preferred method for building the structure.

Users can either use parameters from **neutron scattering data** or input their own parameters derived from density functional theory (DFT) or molecular mechanics (MM) simulations (Figure 4). For detailed experimental crystallographic information, user can check these two references (2, 3).

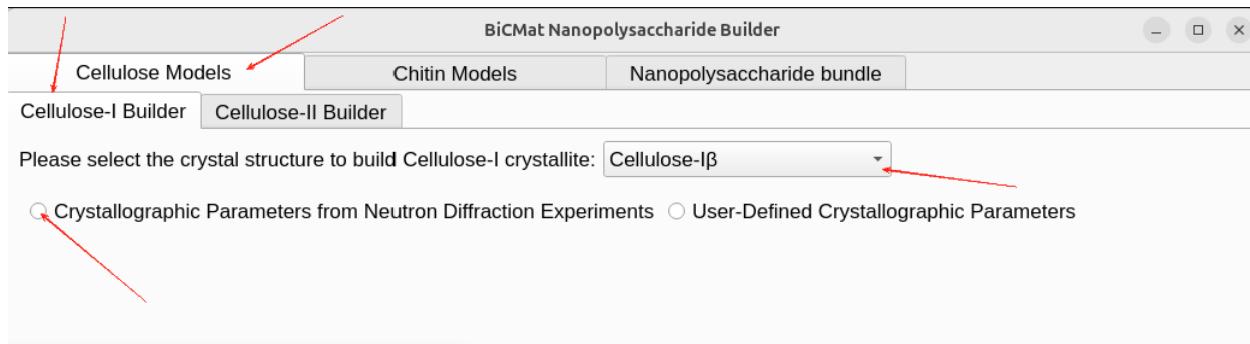


Figure 4

Step 2. Use the drop-down menu to select the desired cross-section. Next, enter the number of **c repetitions** to define the **length of the cellulose structure in the axial direction**. For hexagonal cross-section cellulose, the cross-sectional area is fixed, so only the length needs to be specified. Finally, choose “**No Modification**” to build the native cellulose structure. (Figure 5)

Cellulose Models Chitin Models Nanopolysaccharide bundle

Cellulose-I Builder Cellulose-II Builder

Please select the crystal structure to build Cellulose-I crystallite: Cellulose-I β

(Crystallographic Parameters from Neutron Diffraction Experiments) (User-Defined Crystallographic Parameters)

18-chain hexagonal cross-section shape

Crystallographic parameters

a (Å) 7.784 b (Å) 8.201 c (Å) 10.38 gamma angle γ (°) 96.5

Cross-section width (Å) Cross-section height (Å)

a repetition b repetition c repetition

(Carboxylation) (Sulfate) (No Modification)

a (exp.)=7.784 Å
b (exp.)=8.201 Å
c (exp.)=10.38 Å
 γ (exp.)=96.5°

Cellulose-I β unit: Glucose

II

Cross-section of hexagonal-shape Cellulose-I β (18-chain model)

(110) crystallographic planes

(1-10) crystallographic planes

Cellulose length

Figure 5

Step 3. Use the drop-down menu to select the desired force field. The NPB package currently supports CHARMM36 and GLYCAM06j. Finally, click the “Generate Structure” button. (Figure 6)

Crystallographic parameters

a (Å) 7.784 b (Å) 8.201 c (Å) 10.38 gamma angle γ (°) 96.5

Cross-section width (Å) Cross-section height (Å)

a repetition b repetition c repetition 10

(Carboxylation) (Sulfate) (No Modification)

Atomistic Simulation Force Field: CHARMM36 Finite Chain Model

Generate Structure

Figure 6

2.1.b. Rectangle Shape

The main steps for building rectangular-shaped cellulose are nearly the same as for the hexagonal cross-section. The only difference is that users need to specify the **a, b, and c crystallographic repetitions** and enter them in the appropriate fields (Figure 7).

Crystallographic Parameters from Neutron Diffraction Experiments User-Defined Crystallographic Parameters

Rectangle cross-section shape

Crystallographic parameters

a (Å) 7.784 b (Å) 8.201 c (Å) 10.38 gamma angle γ (°) 96.5

Cross-section width (Å) Cross-section height (Å)

a repetition b repetition c repetition

Carboxylation Sulfate No Modification

Atomistic Simulation Force Field:

Please select the force field for atomistic simulations

- CHARMM36 Infinite Chain Model
- CHARMM36 Finite Chain Model**
- GLYCAM06 Infinite Chain Model
- GLYCAM06 Finite Chain Model

Generate

a (exp.)=7.784 Å
b (exp.)=8.201 Å
c (exp.)=10.38 Å
 γ (exp.)=96.5°

Cellulose-I β unit: Glucose

II

b

a

γ

90°

Cross-section of rectangle-shape Cellulose-I β (arbitrary-chain model)

Cellulose length

(100) crystallographic planes

Figure 7

2.1.c. Parallelogram Shape

The main steps for building parallelogram-shaped cellulose are similar to those for the previous two examples. The difference is that users need to specify the **width, height, and the number of c crystallographic repetitions**, and enter them in the appropriate fields (Figure 8).

Crystallographic Parameters from Neutron Diffraction Experiments User-Defined Crystallographic Parameters

Parallelogram cross-section shape

Crystallographic parameters

a (Å) 7.784 b (Å) 8.201 c (Å) 10.38 gamma angle γ (°) 96.5

Cross-section width (Å) Cross-section height (Å)

a repetition b repetition c repetition

Carboxylation Sulfate No Modification

Atomistic Simulation Force Field:

Please select the force field for atomistic simulations

- CHARMM36 Infinite Chain Model
- CHARMM36 Finite Chain Model**
- GLYCAM06 Infinite Chain Model
- GLYCAM06 Finite Chain Model

Generate

a (exp.)=7.784 Å
b (exp.)=8.201 Å
c (exp.)=10.38 Å
 γ (exp.)=96.5°

Cellulose-I β unit: Glucose

II

Width

γ

b

Height

a

90°

Cross-section of parallelogram-shape Cellulose-I β

Cellulose length

(110) crystallographic planes

Figure 8

2.2. Modified Cellulose

The main steps for building **TEMPO-oxidized** cellulose are similar to those for constructing native cellulose structures. When the **carboxylation ratio** (TEMPO oxidation) option is activated, users need to **specify which cellulose faces** should be modified (Figure 9). The crystallographic faces available for modification will vary depending on the chosen **cross-sectional shape**. For example, in the case of the **parallelogram shape** (representing tunicate cellulose), users can specify the **left and right faces** for modification, as cellulose in this form is not deposited strictly along crystallographic faces. Additionally, users should provide the **surface charge density** and **pH** (Figure 10), which can be set according to their experimental data.

Currently, **only carboxylation** and **half-ester sulfate** modifications are supported for both cellulose I α and I β . **Carboxylation** is compatible with both the CHARMM36 and GLYCAM06j force fields, while **half-ester sulfate** is supported only with the CHARMM36 force field.

Cellulose-I Builder Cellulose-II Builder

Please select the crystal structure to build Cellulose-I crystallite: **Cellulose-I β**

Crystallographic Parameters from Neutron Diffraction Experiments User-Defined Crystallographic Parameters

18-chain hexagonal cross-section shape

Crystallographic parameters

a (\AA) 7.784 b (\AA) 8.201 c (\AA) 10.38 gamma angle γ ($^{\circ}$) 96.5

Cross-section width (\AA) Cross-section height (\AA)

a repetition b repetition c repetition

Carboxylation Sulfate No Modification

Please select cellulose-I β plane for carboxylation modifications:

Surface charge density (unit: mmol/g):

Atomistic Simulation Force Field:

Generate Structure

(110) crystallographic planes

(1-10) crystallographic planes

90°

Cellulose length

Cross-section of hexagonal-shape Cellulose-I β (18-chain model)

II

a (exp.)=7.784 \AA
b (exp.)=8.201 \AA
c (exp.)=10.38 \AA
 γ (exp.)=96.5°

Crystallographic parameter reference: Nishiyama et al. Journal of the American Chemical Society. 2002;124(31):9074-82.

Figure 9

Please select cellulose-I β plane for carboxylation modifications:

Both (1-10) and (110) planes (Only support hexagonal and square cross-section)

Surface charge density (unit: mmol/g): 1.2

Atomistic Simulation Force Field:

CHARMM36 Finite Chain Model

Generate Structure

pH level of cellulose-I β structure (>0 and <14): 7

Figure 10

3. Construction of Chitin Nanostructures

3.1. Native Chitin

Atomic force microscopy (AFM) and transmission electron microscopy (TEM) studies on crustacean cuticles and algal chitin indicate that α -chitin nanofibrils often exhibit a hexagonal-shaped cross section. For β -chitin, diatoms and tubeworms display two distinct cross-sectional shapes: the former typically has a square (rectangular) cross section, while the latter features a parallelogram shape. With NPB, users can generate chitin allomorphs with customized biochemical topologies. Additionally, NPB supports the construction of α - and β -chitin supercells based on unit crystallographic parameters. Below are four examples demonstrating the construction of native chitin nanostructures with different cross-sectional shapes.

3.1.a. Hexagonal Shape (α -chitin)

Step 1. Select the “Chitin Models” and “ α -chitin Builder” buttons, then use the drop-down menu to choose α -chitin-A, α -chitin-B, or α -chitin-AB. In this context, “-A,” “-B,” and “-AB” indicate that all hydroxymethyl groups at the C₆ position are in the “all gg,” “all gt,” or a “mixture of gg and gt at a 0.5:0.5 ratio,” respectively. For more details, please refer to this reference (4).

Next, select your preferred method for building the structure. Users can either use parameters from X-ray diffraction data or input parameters derived from density functional theory (DFT) or molecular mechanics (MM) simulations (Figure 11). For detailed experimental crystallographic information, refer to the provided reference (5).

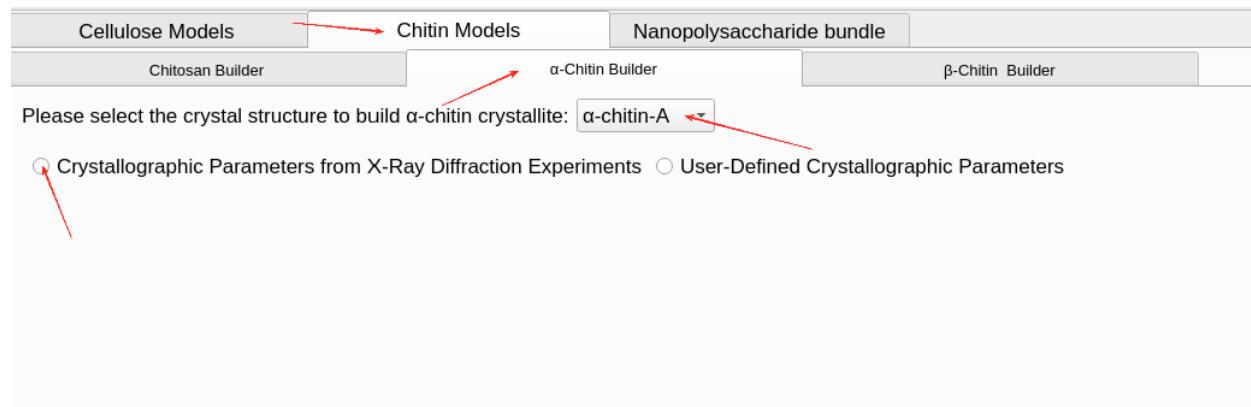


Figure 11

Step 2. Use the drop-down menu to select the desired cross-section. Next, specify the **width**, **height**, and the **number of c crystallographic repetitions**, and enter them in the appropriate fields (Figure 12). Then, choose “**No Modification**” to build the native chitin structure.

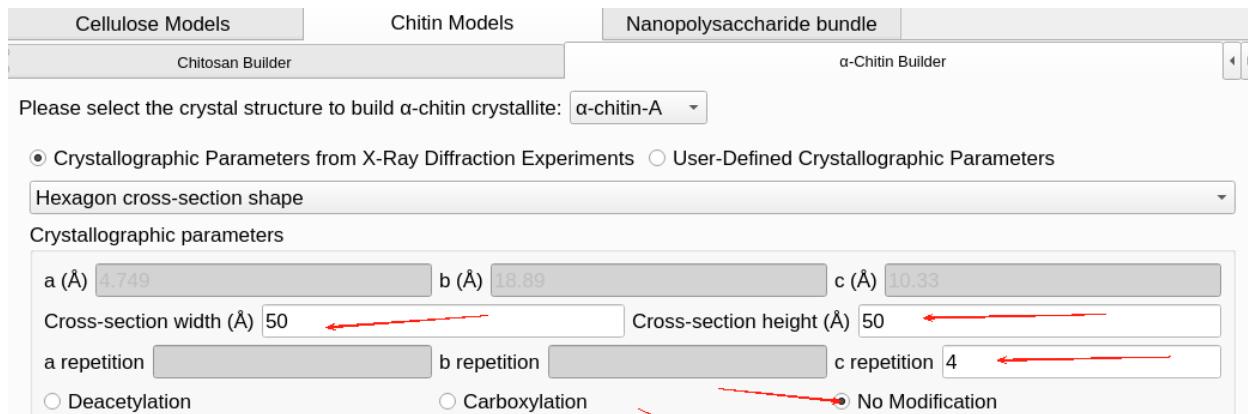


Figure 12

Step 3. Use the drop-down menu to select the desired force field. The NPB package currently supports CHARMM36 and GLYCAM06j for α-chitin native structure. Finally, click the “Generate Structure” button. (Figure 13)

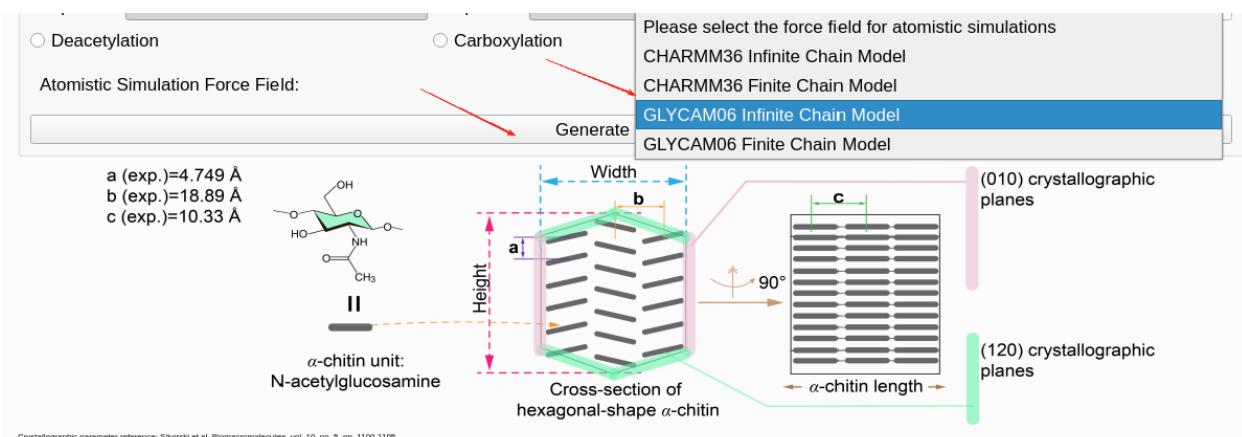


Figure 13

3.1.b. Rectangle Shape (α -chitin)

The main steps for building rectangular-shaped chitin are nearly the same as those for the hexagonal cross-section. The only difference is that users must specify the **a**, **b**, and **c** **crystallographic repetitions** and enter them in the appropriate fields (Figure 14). This method can be used to construct supercell structures of α -chitin crystals based on unit cell crystallographic direction.

The screenshot shows the NPB software interface for building α -chitin crystallites. Key parameters displayed are:

- Crystallographic Parameters from X-Ray Diffraction Experiments:** Selected for this build.
- Rectangle cross-section shape:** Chosen for the build.
- Crystallographic parameters:**
 - a (Å):** 4.749
 - b (Å):** 18.89
 - c (Å):** 10.33
- Cross-section width (Å):** 18.89 Å
- Cross-section height (Å):** 10.33 Å
- a repetition:** 1
- b repetition:** 1
- c repetition:** 1
- Deacetylation:** Unselected.
- Carboxylation:** Unselected.
- No Modification:** Selected.
- Atomistic Simulation Force Field:** CHARMM36 Finite Chain Model

Below the interface, a chemical structure of the α -chitin unit (N-acetylglucosamine) is shown, labeled "II". A diagram illustrates the rectangle-shaped crystal structure with axes **a**, **b**, and **c**. The **a** axis is vertical, **b** is horizontal, and **c** is depth. A 90° rotation arrow is shown between **b** and **c**. The diagram also labels "(010) crystallographic planes" and "(100) crystallographic planes".

Figure 14

3.1.c. Rectangle Shape (β -Chitin: Anhydrous/Dihydrous Configurations)

For β -chitin, both **dihydrous** and **anhydrous** configurations are available (Figure 15). NPB allows users to generate structures in either configuration. Rectangular cross-section morphologies (or supercell structures) can be built by specifying the **a**, **b**, and **c** crystallographic repetitions and entering them in the appropriate fields (Figure 16).

The screenshot shows the NPB software interface for building β -chitin crystallites. The key feature highlighted is the dropdown menu for selecting the crystal structure, which offers three options:

- Select here
- Anhydrous state (highlighted in blue)
- Dihydrous state

Figure 15

Please select the crystal structure to build β -chitin crystallite: Anhydrous state

Crystallographic Parameters from Neutron Diffraction Experiments User-Defined Crystallographic Parameters

Rectangle cross-section shape

Crystallographic parameters

a (\AA)	4.82	b (\AA)	9.24	c (\AA)	10.384	gamma angle γ ($^{\circ}$)	97.16
Cross-section height (010 length) (\AA)		Cross-section width (1-20 length) (\AA)					
a repetition		b repetition		c repetition			

Deacetylation Carboxylation No Modification

Atomistic Simulation Force Field:

Please select the force field for atomistic simulations

Generate Structure

Figure 16

3.1.d. Parallelogram Shape (β -Chitin: Anhydrous/Dihydrous Configurations)

β -chitin structures with parallelogram-shaped cross sections can also be built in both dihydrous and anhydrous configurations. NPB enables users to generate these configurations by specifying the width, height, and **c** crystallographic repetitions, and entering them in the appropriate fields (Figure 17). For more information on dihydrous and anhydrous forms of β -chitin, users are referred to this relevant reference (6).

Please select the crystal structure to build β -chitin crystallite: Anhydrous state

Crystallographic Parameters from Neutron Diffraction Experiments User-Defined Crystallographic Parameters

Parallelogram cross-section shape

Crystallographic parameters

a (\AA)	4.82	b (\AA)	9.24	c (\AA)	10.384	gamma angle γ ($^{\circ}$)	97.16
Cross-section height (010 length) (\AA)		Cross-section width (1-20 length) (\AA)					
a repetition		b repetition		c repetition			

Deacetylation Carboxylation No Modification

Atomistic Simulation Force Field:

Please select the force field for atomistic simulations

Generate Structure

Chemical Structure: β -chitin unit: N-acetylglucosamine (II). The structure shows the repeating unit with its chemical components: a glucose ring, an acetyl group (-CH₃), and an amide linkage (-NH-C(=O)-). The unit II is shown below.

Diagram: A diagram illustrating the cross-section of a parallelogram-shaped β -chitin crystallite. It shows the unit cell with dimensions: Height, Width, and γ (gamma angle). The **c** axis is indicated along the vertical height. A 90° angle is shown between the **c** axis and the **a** axis. To the right, a 3D representation shows the crystallite's structure with (010) crystallographic planes and (1-20) crystallographic planes. The β -chitin length is also indicated.

Crystallographic parameter reference: Nishiyama et al. Macromolecules. 2011;44(4):950-7.
Crystallographic parameter reference: Sawada et al. Biomacromolecules. 2012;13:288-291.

Figure 17

3.2. Modified Chitin

The main steps for building chemically modified chitin are similar to those used for constructing native chitin. Currently, NPB supports both **deacetylation** and **TEMPO-oxidation** modifications for chitin structures. Users must specify which crystallographic faces of the chitin should be modified (Figure 18), and the available modification faces depend on the selected cross-sectional shape.

Additionally, users should provide the **surface charge density** or **deacetylation degree** and pH values, which can be set based on experimental data. For deacetylation, the degree of deacetylation should range from 0 to 1 (Figure 19). For carboxylation, the surface charge can be randomly assigned. Both two chemical modifications will only be applied to exterior chains.

Currently, only carboxylation and half-ester sulfate modifications are supported for both α - and β -chitin. **Carboxylation** and **deacetylation** are compatible with the CHARMM36 force field. However, surface modifications **are not currently supported** with the GLYCAM06j force field for chitin nanostructures.

Please select the crystal structure to build α -chitin crystallite:

Crystallographic Parameters from X-Ray Diffraction Experiments User-Defined Crystallographic Parameters

Rectangle cross-section shape

Crystallographic parameters

a (Å) [4.749] b (Å) [18.89] c (Å) [10.33]

Cross-section width (Å) Cross-section height (Å)

a repetition b repetition c repetition

Deacetylation Carboxylation No Modification

Please select α -chitin plane for deacetylation modifications:

Degree of deacetylation (≥ 0 and < 1):

Atomistic Simulation Force Field:

Crystallographic parameter reference: Sikorski et al. Biomacromolecules, vol. 10, no. 5, pp. 1100-1105.

Diagram illustrating the α -chitin unit: N-acetylglucosamine. It shows the chemical structure of the unit and its cross-section as a rectangle labeled 'Cross-section of rectangle-shape α -chitin'. The rectangle has dimensions 'a' and 'b'. The length of the unit is labeled ' α -chitin length'. A legend indicates '(100) crystallographic planes'.

Select here

- Single (010) plane
- Two (010) planes
- Single (100) plane (Only support rectangle cross-section)
- Two (100) planes (Only support rectangle cross-section)
- Single (100) and (010) planes (Only support rectangle cross-section)
- Both (100) and (010) planes (Only support rectangle cross-section)
- Single (120) plane (Only support hexagon cross-section)
- Two (120) planes (Only support hexagon cross-section)
- Single (120) and (010) planes (Only support hexagon cross-section)
- Both (120) and (010) planes (Only support hexagon cross-section)
- Inside the α -chitin

Figure 18

Deacetylation Carboxylation No Modification

Please select α -chitin plane for deacetylation modifications:

Degree of deacetylation (≥ 0 and < 1):

Atomistic Simulation Force Field:

pH level of α -chitin structure (> 0 and < 14):

CHARMM36 Infinite Chain Model

Figure 19

4. Construction of Nanopolysaccharide Bundles

NPB currently supports the construction of **cellulose I β** bundle structures in both **seven-** and **four-crystallite** configurations. Users can define the inter-fibril distance and bundle length to generate the desired cellulose bundle structure (Figure 20).

For four-crystallite bundles, users can build either **antiparallel** or **parallel** configurations to study inter-fibril fusion dynamics (Figure 21), as demonstrated in our accompanying NPB paper. At present, only cellulose bundle models are supported. **Chitin bundle** modeling is under active development, and future versions of NPB will incorporate more direct tools for constructing chitin bundles.

Figure 20

Figure 21

5. Construction of User-Defined Nanopolysaccharide Structures

In some cases, users may need to use custom-modified structures to study specific properties of nanopolysaccharides—for example, mechanical responses (7). Additionally, to optimize force field parameters, users may need to work with relaxed structures in order to fine-tune interaction terms, such as Lennard-Jones (LJ) parameters (8), during simulations. For these purposes, NPB allows users to build and import their own atomic configurations, with support for both CHARMM36 and GLYCAM06j formats. Users should follow the steps below to build such structures:

Step 1. To ensure smooth integration of user-defined initial configurations with NPB, the input structure should be provided in a **two-sugar-ring** unit in “**pdb**” format. The atom and residue sequence must follow the conventions of either CHARMM36 or GLYCAM06j, as illustrated in Figure 22.

ATOM	1	C1	BGLC	1	12.669	12.493	-0.137	1.00	0.00	C
ATOM	2	H1	BGLC	1	12.806	13.068	0.647	1.00	0.00	H
ATOM	3	C5	BGLC	1	10.889	11.258	0.920	1.00	0.00	C
ATOM	4	H5	BGLC	1	10.985	11.749	1.761	1.00	0.00	H
ATOM	5	O5	BGLC	1	12.153	11.223	0.242	1.00	0.00	O
ATOM	6	C2	BGLC	1	11.723	13.135	-1.146	1.00	0.00	C
ATOM	7	H2	BGLC	1	11.623	12.562	-1.934	1.00	0.00	H
ATOM	8	O2	BGLC	1	12.278	14.398	-1.514	1.00	0.00	O
ATOM	9	H02	BGLC	1	13.198	14.271	-1.209	1.00	0.00	H
ATOM	10	C3	BGLC	1	10.386	13.310	-0.452	1.00	0.00	C
ATOM	11	H3	BGLC	1	10.500	13.911	0.312	1.00	0.00	H
ATOM	12	O3	BGLC	1	9.469	13.893	-1.372	1.00	0.00	O
ATOM	13	H03	BGLC	1	8.718	14.066	-0.778	1.00	0.00	H
ATOM	14	C4	BGLC	1	9.873	11.962	0.042	1.00	0.00	C
ATOM	15	H4	BGLC	1	9.677	11.398	-0.733	1.00	0.00	H
ATOM	16	O4	BGLC	1	8.676	12.109	0.825	1.00	0.00	O
ATOM	17	C6	BGLC	1	10.518	9.820	1.214	1.00	0.00	C
ATOM	18	H61	BGLC	1	10.256	9.375	0.395	1.00	0.00	H
ATOM	19	H62	BGLC	1	11.293	9.354	1.573	1.00	0.00	H
ATOM	20	O6	BGLC	1	9.468	9.754	2.150	1.00	0.00	O
ATOM	21	H06	BGLC	1	9.768	8.997	2.681	1.00	0.00	H
ATOM	22	C1	BGLC	2	7.472	11.806	0.163	1.00	0.00	C
ATOM	23	H1	BGLC	2	7.583	11.251	-0.599	1.00	0.00	H
ATOM	24	C5	BGLC	2	5.689	13.071	-0.920	1.00	0.00	C
ATOM	25	H5	BGLC	2	5.793	12.557	-1.752	1.00	0.00	H
ATOM	26	O5	BGLC	2	6.946	13.131	-0.231	1.00	0.00	O
ATOM	27	C2	BGLC	2	6.518	11.277	1.238	1.00	0.00	C
ATOM	28	H2	BGLC	2	6.461	11.886	1.993	1.00	0.00	H
ATOM	29	O2	BGLC	2	7.056	10.823	1.645	1.00	0.00	O
ATOM	30	H02	BGLC	2	7.867	10.311	2.103	1.00	0.00	H
ATOM	31	C3	BGLC	2	5.164	11.112	0.599	1.00	0.00	C
ATOM	32	H3	BGLC	2	5.219	10.430	-0.106	1.00	0.00	H
ATOM	33	O3	BGLC	2	4.266	10.653	1.014	1.00	0.00	O
ATOM	34	H03	BGLC	2	3.418	11.002	1.235	1.00	0.00	H
ATOM	35	C4	BGLC	2	4.675	12.409	-0.016	1.00	0.00	C
ATOM	36	H4	BGLC	2	4.469	13.028	0.714	1.00	0.00	H
ATOM	37	O4	BGLC	2	3.488	12.243	-0.799	1.00	0.00	O
ATOM	38	C6	BGLC	2	5.330	14.522	-1.241	1.00	0.00	C
ATOM	39	H61	BGLC	2	5.068	14.979	-0.428	1.00	0.00	H
ATOM	40	H62	BGLC	2	6.100	14.978	-1.615	1.00	0.00	H
ATOM	41	O6	BGLC	2	4.265	14.539	-2.171	1.00	0.00	O
ATOM	42	H06	BGLC	2	4.717	14.928	-2.938	1.00	0.00	H
ATOM	1	C1	4GB	1	12.669	12.493	-0.137	1.00	0.00	C
ATOM	2	H1	4GB	1	12.806	13.068	0.647	1.00	0.00	H
ATOM	3	O5	4GB	1	12.153	11.223	0.242	1.00	0.00	O
ATOM	4	C5	4GB	1	10.889	11.258	0.920	1.00	0.00	C
ATOM	5	H5	4GB	1	10.985	11.749	1.761	1.00	0.00	H
ATOM	6	C6	4GB	1	10.518	9.820	1.214	1.00	0.00	C
ATOM	7	H61	4GB	1	10.256	9.375	0.395	1.00	0.00	H
ATOM	8	H62	4GB	1	11.293	9.354	1.573	1.00	0.00	H
ATOM	9	O6	4GB	1	9.469	9.754	2.150	1.00	0.00	O
ATOM	10	H60	4GB	1	9.768	8.997	2.681	1.00	0.00	H
ATOM	11	C4	4GB	1	9.873	11.962	0.042	1.00	0.00	C
ATOM	12	H4	4GB	1	9.677	11.398	-0.733	1.00	0.00	H
ATOM	13	C3	4GB	1	10.386	13.310	-0.452	1.00	0.00	C
ATOM	14	H3	4GB	1	10.500	13.911	0.312	1.00	0.00	H
ATOM	15	O3	4GB	1	9.469	13.893	-1.372	1.00	0.00	O
ATOM	16	H30	4GB	1	8.718	14.066	-0.778	1.00	0.00	H
ATOM	17	C2	4GB	1	11.723	13.135	-1.146	1.00	0.00	C
ATOM	18	H2	4GB	1	11.623	12.562	-1.934	1.00	0.00	H
ATOM	19	O2	4GB	1	12.278	14.398	-1.514	1.00	0.00	O
ATOM	20	H20	4GB	1	13.198	14.271	-1.209	1.00	0.00	H
ATOM	21	O4	4GB	1	8.676	12.109	0.825	1.00	0.00	O
ATOM	22	C1	4GB	2	7.472	11.860	0.163	1.00	0.00	C
ATOM	23	H1	4GB	2	7.583	11.251	-0.599	1.00	0.00	H
ATOM	24	O5	4GB	2	6.946	13.131	-0.231	1.00	0.00	O
ATOM	25	C5	4GB	2	5.689	13.071	-0.920	1.00	0.00	C
ATOM	26	H5	4GB	2	5.793	12.557	-1.752	1.00	0.00	H
ATOM	27	C6	4GB	2	5.330	14.522	-1.241	1.00	0.00	C
ATOM	28	H61	4GB	2	5.068	14.979	-0.428	1.00	0.00	H
ATOM	29	H62	4GB	2	6.100	14.978	-1.615	1.00	0.00	H
ATOM	30	O6	4GB	2	4.265	14.539	-2.171	1.00	0.00	O
ATOM	31	H60	4GB	2	4.717	14.928	-2.938	1.00	0.00	H
ATOM	32	C4	4GB	2	4.675	12.409	-0.016	1.00	0.00	C
ATOM	33	H4	4GB	2	4.469	13.028	0.714	1.00	0.00	H
ATOM	34	C3	4GB	2	5.164	11.112	0.599	1.00	0.00	C
ATOM	35	H3	4GB	2	5.219	10.430	-0.106	1.00	0.00	H
ATOM	36	O3	4GB	2	4.266	10.653	1.614	1.00	0.00	O
ATOM	37	H30	4GB	2	3.418	11.002	1.235	1.00	0.00	H
ATOM	38	C2	4GB	2	6.518	11.277	1.230	1.00	0.00	C
ATOM	39	H2	4GB	2	6.461	11.866	1.993	1.00	0.00	H
ATOM	40	O2	4GB	2	7.056	10.823	1.645	1.00	0.00	O
ATOM	41	H20	4GB	2	7.867	10.311	2.183	1.00	0.00	H
ATOM	42	O4	4GB	2	3.488	12.243	-0.799	1.00	0.00	O

Figure 22. PDB file sequence of a cellobiose unit: left in CHARMM36 format, and right in GLYCAM06j format.

Step 2. Users need to name the unit structure using a predefined format and place it in the designated directory. All required details are provided in Table 1.

Table 1

Naonpolysaccharide Type	Force Field	PDB File Name	4 th Column Variable Name (in PDB file)	5 th Column Variable Name (in PDB file)
Cellulose I α	CHARMM36	chain_ud.pdb	BGLC	1, 2
Cellulose I α (Finite model)	GLYCAM06j	chain-finite_ud.pdb	4GB	2, 3
Cellulose I α (Infinite model)	GLYCAM06j	chain_ud.pdb	4GB	1, 2
Cellulose I β	CHARMM36	chain-1_ud.pdb chain-2_ud.pdb	BGLC	1, 2
Cellulose I β (Finite model)	GLYCAM06j	chain-1-finite_ud.pdb chain-2-finite_ud.pdb	4GB	2, 3
Cellulose I β (Infinite model)	GLYCAM06j	chain-1_ud.pdb chain-2_ud.pdb	4GB	1, 2
α -chitin	CHARMM36	left-unit_ud.pdb right-unit_ud.pdb	BLNAN	1, 2
α -chitin (Finite model)	GLYCAM06j	left-unit-finite_ud.pdb right-unit-finite_ud.pdb	4YB	2, 3
α -chitin (Infinite model)	GLYCAM06j	left-unit_ud.pdb right-unit_ud.pdb	4YB	1, 2
β -chitin (Anhydrous)	CHARMM36	unit-ud.pdb	BLNA	1, 2
β -chitin (Dihydrous)	CHARMM36	dihydrous-unit-ud.pdb	BDNA	1, 2
β -chitin (Anhydrous; Finite)	GLYCAM06j	unit-ud-finite.pdb	4YB	2, 3
β -chitin (Anhydrous; Infinite)	GLYCAM06j	unit-ud.pdb	4YB	1,2

Note: For cellulose I α , NPB requires only a single unit structure. Users can refer to the original (experimentally based) structure file located at “./npb_dev1/structure/cellulose_I_alpha” for details—particularly the chain polarity.

For cellulose I β and α -chitin, users must provide two chain units. Additional information can be found in the ./npb_dev1/structure directory.

For β -chitin, NPB currently supports both anhydrous and dihydrus configurations in the CHARMM36 format. Users should note that the dihydrus form includes four additional water

molecules per unit. Further details can be found in “./npb_dev1/structure/beta_chitin”. The GLYCAM06j force field currently supports β -chitin only in the anhydrous form.

Note: For the CHARMM36 force field, residue names do not need to distinguish between non-reducing and reducing ends. Therefore, for the two-sugar unit, users should simply set the resid numbers to 1 and 2 (**the 5th column number in the PDB file**). The file name should be “**xxx_ud.pdb**” and placed in the required structure folder within the “./npb_dev1/structure/xxx/charmm” directory.

For the **GLYCAM06j** force field, the structure includes a reducing end (ROH) to construct a **finite-length nanopolysaccharide**. When preparing the two-sugar units for GLYCAM06j, users should **start the resid numbering from 2 to 3**(**the 5th column number in the PDB file**). Additionally, the file should be named “**xxx-finite_ud.pdb**”, as listed in Table 1. For infinite structure, the file name should be “**xxx_ud.pdb**”. The unit structure files should be placed in the required structure folder within the “./npb_dev1/structure/xxx/glycam” directory.

Once users have built their own unit sugar rings, they can place them in the designated location as previously described. Alternatively, users may use experimental unit structures with customized crystallographic parameters. Both self-built and experimental units are acceptable. If a user does not provide a custom unit structure, NPB will default to the experimental structure.

As shown in Figure 23 left image, we demonstrate the process of building a customized cellulose-I α structure (18-chain hexagonal shape). Users need to complete all required fields to build the structure.

If the crystallographic parameters entered are inappropriate, NPB will prompt the user, suggesting that the parameters are not proper (Figure 23 right image). In such cases, users can refer to the experimental data—displayed at the bottom of the GUI interface—as a guide to fine-tune the parameters.

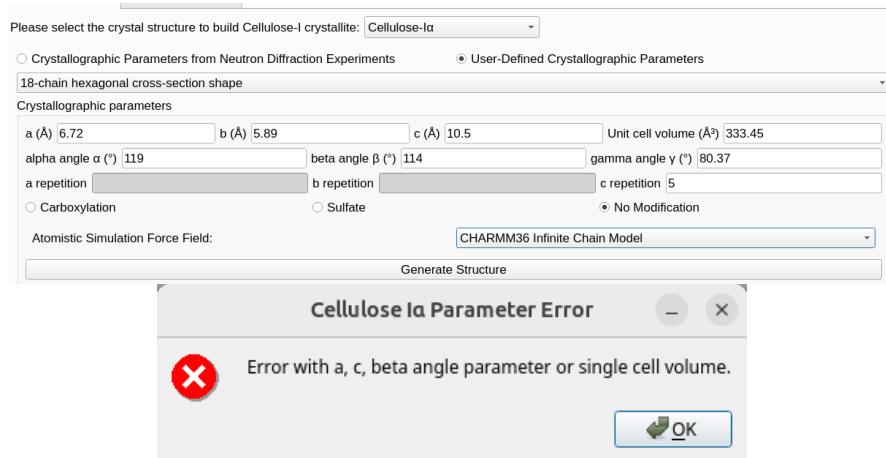


Figure 23

6. Examples of Using NPB-Generated Files for Molecular Dynamics (MD) Simulations

To help users make the most of NPB-generated files, we present three examples that incorporate different MD engines: NAMD, AMBER, and GROMACS. Detailed example files are provided in the “`./NPB_dev1/simulation/`”.

6.1. TEMPO-Oxidized Cellulose-I α

In this example, we used NPB to produce a cellulose-I α structure (18-chain hexagonal cross-section shape) with a surface charge density of 1.2 mmol/g carboxyl groups. The files are generated using CHARMM36 force field, which can be used to run MD simulation by using NAMD. All necessary files are provided in the “`./NPB_dev1/simulation/namd`” directory.

If users wish to run simulations in the dry state, the generated files can be used directly—simply update the first two lines in “`eq.conf`” to reference “`cellulose.pdb`” and “`cellulose.psf`,” and disable the barostat in “`eq.conf`” (see Figure 22). However, this approach is not recommended, as TEMPO-oxidized cellulose possesses surface charges that require counterions for neutralization in a solution environment. Users can use **VMD** by opening the “**TK Console**” and typing “`source solvate.tcl`” to generate the cellulose structure in water with counterions.

```
##temperature and pressure
langevin          on
langevinDamping   1
langevinTemp      300.0
langevinHydrogen  no
langevinpiston    on    #####off for NVT
langevinpistontarget 1.01325
langevinpistonperiod 200
langevinpistondecay 100
langevinpistontemp  300.0
usegrouppressure  yes  #####no for NVT
```

Figure 22.

Users can run the simulation by first downloading NAMD3 and navigating to the case directory. Simply enter the following commands (see the `README.md` file in this folder for more details):

```
1 /PATH/TO/NAMD/namd3 +p12 +idlepoll eq.conf
2
3 /PATH/TO/NAMD/namd3 +p12 +idlepoll md.conf
```

6.2. TEMPO-Oxidized Cellulose- $\text{I}\beta$

In this example, we used NPB to generate a cellulose- $\text{I}\beta$ structure (36-chain square cross-section) with a surface charge density of 1.2 mmol/g carboxyl groups. The files were generated using the GLYCAM06j force field and are suitable for running MD simulations with AMBER. All necessary files are available in the “./NPB_dev1/simulation/amber” directory.

We recommend that users solvate the structure and include counterions before running MD simulations. A provided Python script (**fcm.py**) allows users to define their own ion types and concentrations according to the AMBER manual (see Figure 24). Before running the script, users should activate the appropriate Python environment containing all required dependencies for the NPB package.

```
##-----adding ions-----
cation_name    = "Na+"
cation_number  = 110

anion_name     = "Cl-"
anion_number   = 13
##-----adding ions-----
```

Figure 24

The complete script for running this example is shown below:

```
01 ##activate conda environment (optional)
02 conda activate npb
03 ###build the structure with solvents
04 python fcm.py
05
06 /path/to/AMBER/pmemd.cuda -O -i em.mdin -o min300.out -p cell_solv.prmtop -c
07 cell_solv.inpcrd -r min300.rst -inf min300.info -ref cell_solv.inpcrd -x
08 min300.mdcrd
09
10 /path/to/AMBER/pmemd.cuda -O -i pr.mdin -o pr.out -p cell_solv.prmtop -c
min300.rst -r pr.rst -inf pr.info -ref min300.rst -x pr.mdcrd

/path/to/AMBER/pmemd.cuda -O -i md.mdin -o md.out -p cell_solv.prmtop -c pr.rst
-r md.rst -inf md.info -ref pr.rst -x md.mdcrd
```

6.3. Antiparallel Arrangement Cellulose-I β bundle

In this example, we used NPB to generate a cellulose-I β bundle with an antiparallel arrangement between neighboring crystallites. The files were generated using the **CHARMM36** force field and are suitable for running MD simulations with NAMD. In this section, however, we use another MD engine, GROMACS, to perform the simulation. All necessary files are provided in the “`./NPB_dev1/simulation/gmx`” directory.

Users can run simulations in both dry and hydrated states (with water). First, use VMD to invoke TopoTools (we recommend version 1.10, which can be downloaded from: <https://github.com/akohlmey/topotools?tab=readme-ov-file>). Typing the following scripts:

```
1 vmd cellulose.psf cellulose.pdb # ("cellulose" can be replaced with any structure name)
2
3 #####open VMD TK/Console
4 package require topotools
5 topo writegmxtop system.top par_all36_carb.prm # "system.top" can be replaced with any desired
6 ##system.top can be replaced with any name
```

After the “`system.top`” file is generated, users can run the simulation directly with GROMACS using the following script:

```
01 gmx editconf -f cellulose.pdb -o system.gro -c -d 2
02
03 gmx grompp -f em.mdp -c system.gro -p system.top -o em.tpr
04 gmx mdrun -v -deffnm em -ntmpi 1 -pin on
05
06 gmx grompp -f pr.mdp -c em.gro -p system.top -o pr.tpr
07 gmx mdrun -v -deffnm pr -ntmpi 1 -pin on
08
09 gmx grompp -f md.mdp -c pr.gro -p system.top -o md.tpr
10 gmx mdrun -v -deffnm md -ntmpi 1 -pin on
```

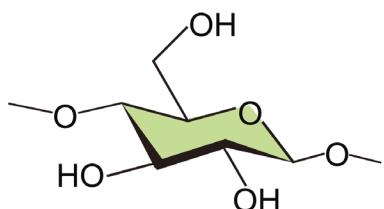
If users wish to perform the simulation in the hydrated state, one additional step is required before running the GROMACS “`grompp`” script mentioned above. A TIP3P-Charmm compatible “`.itp`” file is also provided in the `gmx` folder.

```
1 gmx solvate -cp cellulose.pdb -cs spc216.gro -p system.top -o em.gro
2
```

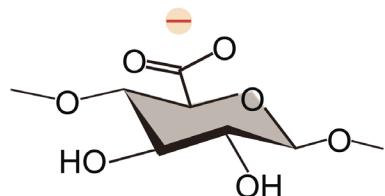
7. Monosaccharide Topologies Utilized in NPB

7.1. CHARMM36 Force Field

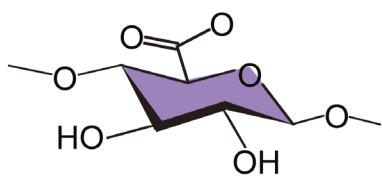
7.1.a Cellulose



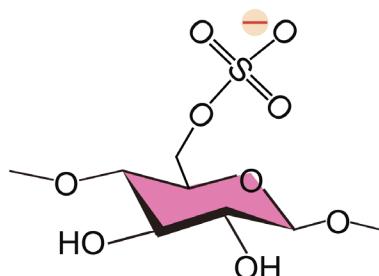
Glucose
Resname : BGLC



Deprotonated Glucuronic Acid
Resname : BGLA



Protonated Glucosamine
Resname : BGLD



Deprotonated glucose-6-sulfate
Resname : BGLS

Figure 24. Monosaccharide used to construct cellulose nanostructures in the CHARMM36 force field.

Table 2.
Atom list of resname BGLC (structure with a net charge of 0)

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	O2	OC311
HO1 (Reduced end)	HCP1	HO2	HCP1
C5	CC3163	C3	CC3161
H5	HCA1	H3	HCA1
O5	OC3C61	O3	OC311
C4	CC3161	HO3	HCP1
H4	HCA1	C6	CC321
O4	OC311	H61	HCA2
HO4 (Non-reduced end)	HCP1	H62	HCA2
O6	OC311	HO6	HCP1

Table 3.
Atom list of resname BGLA (structure with a net charge of -1)

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	O2	OC311
HO1 (Reduced end)	HCP1	HO2	HCP1
C5	CC3163	C3	CC3161
H5	HCA1	H3	HCA1
O5	OC3C61	O3	OC311
C4	CC3161	HO3	HCP1
H4	HCA1	C6	CC202
O4	OC311	O61	OC2D2
HO4 (Non-reduced end)	HCP1	O62	OC2D2

Table 4.
Atom list of resname BGLD (structure with a net charge of 0)

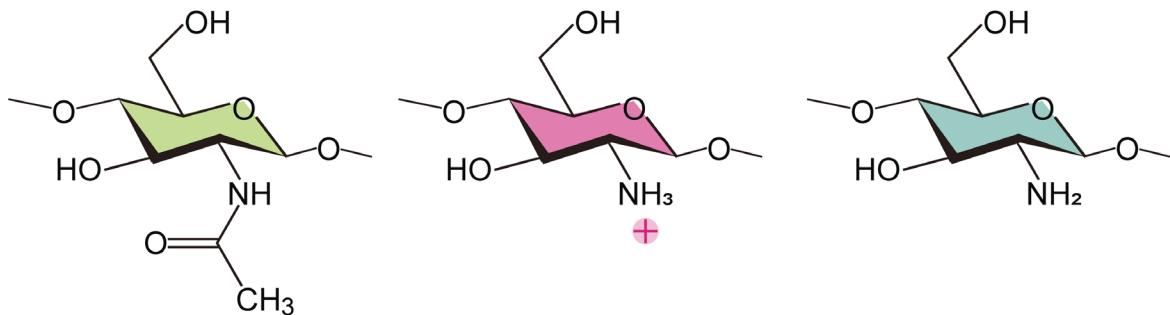
Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	O2	OC311
HO1 (Reduced end)	HCP1	HO2	HCP1
C5	CC3163	C3	CC3161
H5	HCA1	H3	HCA1
O5	OC3C61	O3	OC311
C4	CC3161	HO3	HCP1
H4	HCA1	C6	CC202
O4	OC311	O61	OC2D2
HO4 (Non-reduced end)	HCP1	O62	OC2D2

Table 5.

Atom list of resname BGLS (structure with a net charge of -1)

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	O2	OC311
HO1 (Reduced end)	HCP1	HO2	HCP1
C5	CC3163	C3	CC3161
H5	HCA1	H3	HCA1
O5	OC3C61	O3	OC311
C4	CC3161	HO3	HCP1
H4	HCA1	C6	CC321
O4	OC311	H61	HCA2
HO4 (Non-reduced end)	HCP1	H62	HCA2
O6	OC30P	S6	SC
OS62	OC2DP	OS62	OC2DP
OS64	OC2DP		

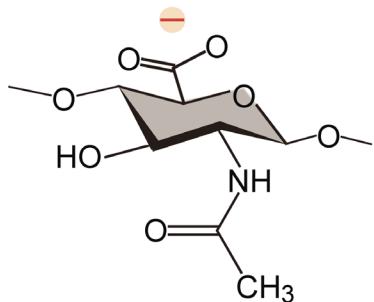
7.1.b Chitin



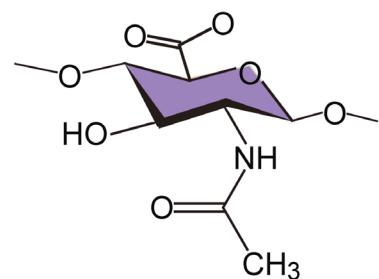
N-Acetylglucosamine
Resname : BLNA

Protonated Glucosamine
Resname : BLNP

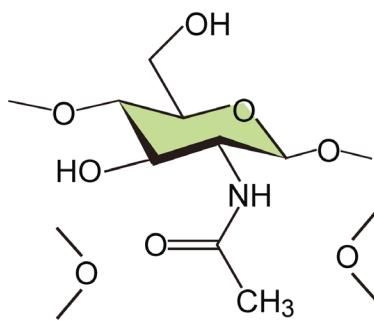
Deprotonated Glucosamine
Resname : BLND



Deprotonated N-acetylglucosaminuronic Acid
Resname : BLCP



Protonated N-acetylglucosaminuronic Acid
Resname : BLCD



Dihydrous N-Acetylglucosamine
Resname : BDNA

Figure 25. Monosaccharide used to construct chitin nanostructures in the CHARMM36 force field.

Table 6.**Atom list of resname BLNA (structure with a net charge of 0)**

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	N	NC2D1
HO1 (Reduced end)	HCP1	HN	HCP1
C5	CC3163	C	CC201
H5	HCA1	O	OC2D1
O5	OC3C61	CT	CC331
C4	CC3161	HT1	HCA3
H4	HCA1	HT2	HCA3
O4	OC311	HT3	HCA3
HO4 (Non-reduced end)	HCP1	C3	CC3161
C6	CC321	H3	HCA1
H61	HCA2	O3	OC311
H62	HCA2	HO3	HCP1
O6	OC311	HO6	HCP1

Table 7.**Atom list of resname BLNP (structure with a net charge of +1)**

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	N	NG3P3
HO1 (Reduced end)	HCP1	HN1	HGP2
C5	CC3163	HN2	HGP2
H5	HCA1	NH3	HGP2
O5	OC3C61	C3	CC3161
C4	CC3161	H3	HCA1
H4	HCA1	O3	OC311
O4	OC311	HO3	HCP1
HO4 (Non-reduced end)	HCP1	HO6	HCP1
C6	CC321	H62	HCA2
H61	HCA2	O6	OC311

Table 8.
Atom list of resname BLND (structure with a net charge of 0)

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	N2	NC2D1
HO1 (Reduced end)	HCP1	HN21	HCP1
C5	CC3163	HN22	HCP1
H5	HCA1	C3	CC3161
O5	OC3C61	H3	HCA1
C4	CC3161	O3	OC311
H4	HCA1	HO3	HCP1
O4	OC311	HO6	HCP1
HO4 (Non-reduced end)	HCP1	H62	HCA2
C6	CC321	O6	OC311
H61	HCA2		

Table 9.
Atom list of resname BLCP (structure with a net charge of -1)

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	N	NC2D1
HO1 (Reduced end)	HCP1	HN	HCP1
C5	CC3163	C	CC201
H5	HCA1	O	OC2D1
O5	OC3C61	CT	CC331
C4	CC3161	HT1	HCA3
H4	HCA1	HT2	HCA3
O4	OC311	HT3	HCA3
HO4 (Non-reduced end)	HCP1	C3	CC3161
C6	CC202	H3	HCA1
O61	OC2D2	O3	OC311
O62	OC2D2	HO3	HCP1

Table 10.
Atom list of resname BLCD (structure with a net charge of 0)

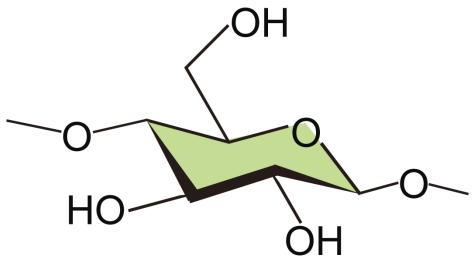
Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	N	NC2D1
HO1 (Reduced end)	HCP1	HN	HCP1
C5	CC3163	C	CC201
H5	HCA1	O	OC2D1
O5	OC3C61	CT	CC331
C4	CC3161	HT1	HCA3
H4	HCA1	HT2	HCA3
O4	OC311	HT3	HCA3
HO4 (Non-reduced end)	HCP1	C3	CC3161
C6	CC202	H3	HCA1
O61	OC2D2	O3	OC311
O62	OC2D2	HO3	HCP1

Table 11.**Atom list of resname BDNA (structure with a net charge of 0)**

Atom	Atomtypes	Atom	Atomtypes
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	N	NC2D1
HO1 (Reduced end)	HCP1	HN	HCP1
C5	CC3163	C	CC201
H5	HCA1	O	OC2D1
O5	OC3C61	CT	CC331
C4	CC3161	HT1	HCA3
H4	HCA1	HT2	HCA3
O4	OC311	HT3	HCA3
HO4 (Non-reduced end)	HCP1	C3	CC3161
C6	CC321	H3	HCA1
H61	HCA2	O3	OC311
H62	HCA2	HO3	HCP1
O6	OC311	HO6	HCP1
OB1	OCTIP3	HB1	HCTIP3
HB2	HCTIP3	OB2	OCTIP3
HB3	HCTIP3	HB4	HCTIP3

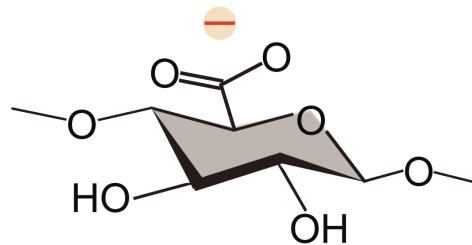
7.2. GLYCAM06j Force Field

7.2.a Cellulose



Glucose

Resname : 4GB/0GB



Deprotonated Glucuronic Acid

Resname : 4ZB/0ZB

Figure 26. Monosaccharide used to construct cellulose nanostructures in the GLYCAM06j force field.

Table 12.

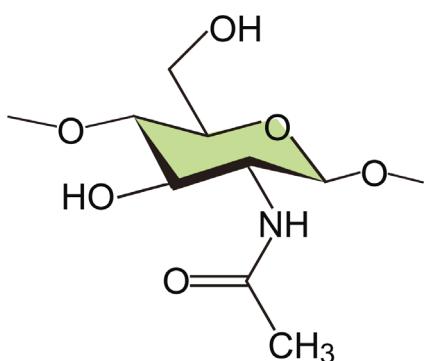
Atom list of resname 4GB/0GB (structure with a net charge of 0)

Atom	Atomtypes	Atom	Atomtypes
C1	Cg	C2	Cg
H1	H2	H2	H1
O1 (Reduced end, ROH)	Ho	O2	Oh
HO1 (Reduced end, ROH)	Oh	H2O	Ho
C5	Cg	C3	Cg
H5	H1	H3	H1
O5	Os	O3	Oh
C4	Cg	H3O	Ho
H4	H1	C6	Cg
O4	Os	H61	H1
H4O (Non-reduced end; 0GB)	Ho	H62	H1
O6	Oh	H6O	Ho

Table 13.**Atom list of resname 4ZB/0ZB (structure with a net charge of -1)**

Atom	Atomtypes	Atom	Atomtypes
C1	Cg	C2	Cg
H1	H2	H2	H1
O1 (Reduced end, ROH)	Ho	O2	Oh
HO1 (Reduced end, ROH)	Oh	H2O	Ho
C5	Cg	C3	Cg
H5	H1	H3	H1
O5	Os	O3	Oh
C4	Cg	H3O	Ho
H4	H1	C6	C
O4	Os	O6B	O2
H4O (Non-reduced end; 0GB)	Ho	O6A	O2
O6	Oh		

7.2.b Chitin



N-Acetylglucosamine
Resname : 4YB/0YB

Figure 27. Monosaccharide used to construct chitin nanostructures in the GLYCAM06j force field.

Table 14.**Atom list of resname 4YB/0YB (structure with a net charge of 0)**

Atom	Atomtypes	Atom	Atomtypes
C1	Cg	C2	Cg
H1	H1	H2	H1
O1 (Reduced end)	Oh	N2	Ng
HO1 (Reduced end)	Ho	H2N	H
C5	Cg	C2N	C
H5	H1	O2N	O
O5	OS	CME	Cg
C4	Cg	H3M	Hc
H4	H1	H2M	Hc
O4	Os/Oh(Non-reduced end)	H1M	Hc
H4O (Non-reduced end)	Ho	C3	Cg
C6	Cg	H3	H1
H61	H1	O3	Oh
H62	H1	H3O	Ho
O6	Oh	H6O	Ho

8. Implementation Details and Algorithms in NPB

8.1 General Logic for Constructing Nanopolysaccharide Structures with NPB

NPB provides a GUI that enables users to select the desired nanopolysaccharide type, morphology, surface chemistry, and force field required to generate nanopolysaccharide structures for atomistic simulations. The detailed workflow is illustrated in Figure 28.

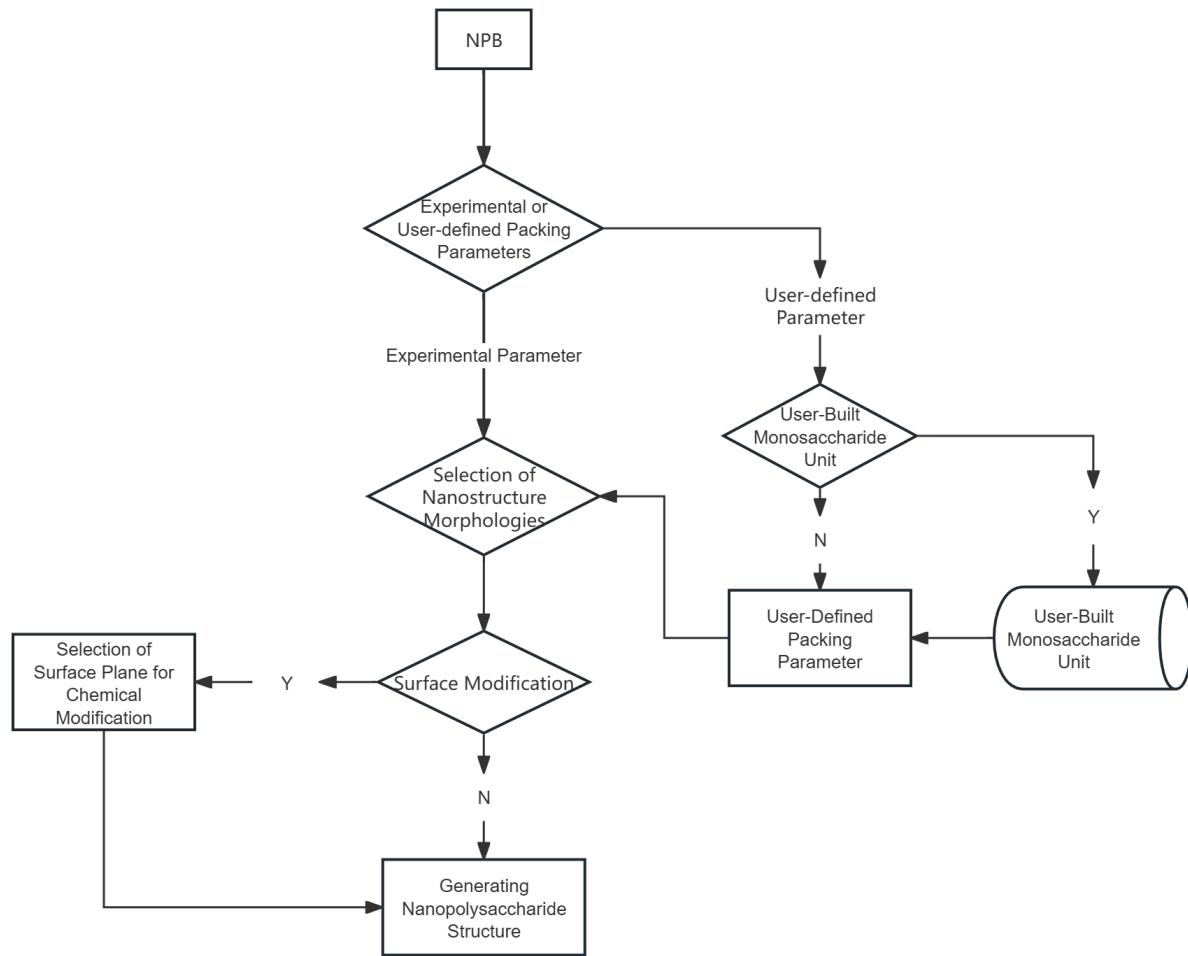


Figure 28. Flowchart of the detailed procedure for building nanopolysaccharide structures with the NPB package.

By using NPB, users can either input direct experimental data or specify their own parameter values to pack polysaccharide polymer chains into nanostructures. When user-defined parameters are employed, NPB also allows users to utilize their own molecular structures, as detailed in Chapter 5. After selecting the parameters for packing the unit cell into nanostructures, users can choose the desired morphology, primarily the cross-sectional shape, to construct nanostructures

that reflect the characteristics of cellulose or chitin from specific natural species. Next, users may opt for surface chemical modification by selecting the surface plane to be chemically modified. Once these choices are made, the nanostructure can be built. The entire process is streamlined and user-friendly, requiring only the input of values, selection of radio buttons, and choice of options from dropdown menus.

8.2 Surface Functionalization Workflow in NPB

NPB enable user to select the arbitrary surface plane to do chemical modifications, where the chemical functional groups of specic chains at the surface are selected to be subsititude with required functional groups. The overall idea is displayed in Figure 29.

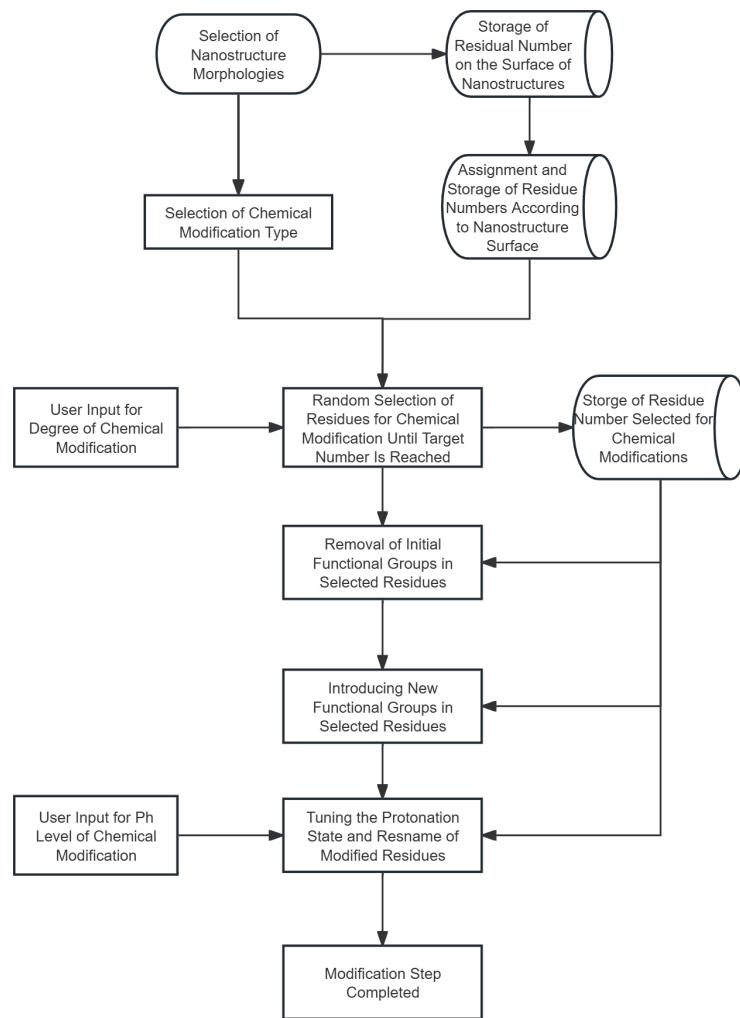


Figure 28. Flowchart of the Detailed Procedure for Surface Modification Implemented in NPB

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