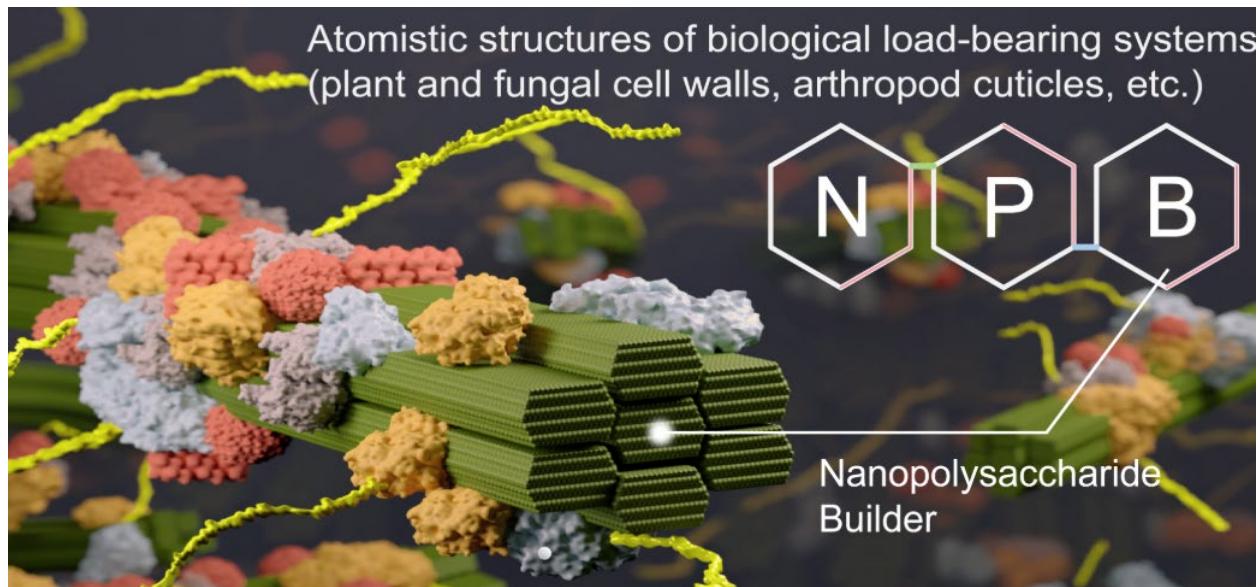


# **Nanopolysaccharide Builder (NPB)**

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

*Zhangmin Wan<sup>a,§</sup>, Yan Yu<sup>b,c,§</sup>, Gio Ferson M. Bautista<sup>d</sup>, Simcha Srebnik<sup>a,\*</sup>, Jeremy C. Smith<sup>c,e,\*</sup>, Orlando J. Rojas<sup>a,d,f,\*</sup>*

<sup>a</sup> Bioproduct Institute, Department of Chemical and Biological Engineering, The University of British Columbia, Vancouver, BC, V6T 1Z3, Canada.

<sup>b</sup> UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

<sup>c</sup> Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

<sup>d</sup> Department of Chemistry, The University of British Columbia, Vancouver, BC V6T 1Z1, Canada.

<sup>e</sup> Department of Biochemistry and Cellular and Molecular Biology, University of Tennessee, Knoxville, Tennessee 37996, United States

<sup>f</sup> Department of Wood Science, The University of British Columbia, Vancouver, BC, V6T 1Z4, Canada.

\*To whom correspondence should be forwarded: orlando.rojas@ubc.ca; smithjc@ornl.gov, simcha.srebnik@ubc.ca

§: These authors contributed equally to this work.

This NPB manual provides guidance on the use of the software package that develops structures and topology files of cellulose and chitin nanostructures. NPB is supported by both **CHARMM36** and **GLYCAM06j** force fields for nanopolysaccharides. Step-by-step instructions are provided to prepare all necessary files for simulations in **NAMD**, **AMBER**, and **GROMACS**.

## **License and Disclaimer**

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The programs and scripts provided in the NPB package are distributed *as is*, without any guarantees or warranties, either expressed or implied. The authors disclaim any responsibility for loss, damage, or malfunction arising from the use of this software.

The NPB tool and its user manual are continuously updated as new features and improvements are implemented. Users are encouraged to check regularly for the latest version.

For questions, suggestions, or to report bugs, please open an issue in the [NPB public repository](#).

## **Citing NPB**

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## 1. NPB Package Installation

The required dependencies for the **Nanopolysaccharide Builder (NPB)** toolkit can be installed using one of the methods outlined below for Unix-like systems (e.g., Ubuntu 24.04). For users operating on **macOS**, a brief installation guide is provided in **Chapter 1.3** of the user manual.

### 1.1 Installation of Ubuntu

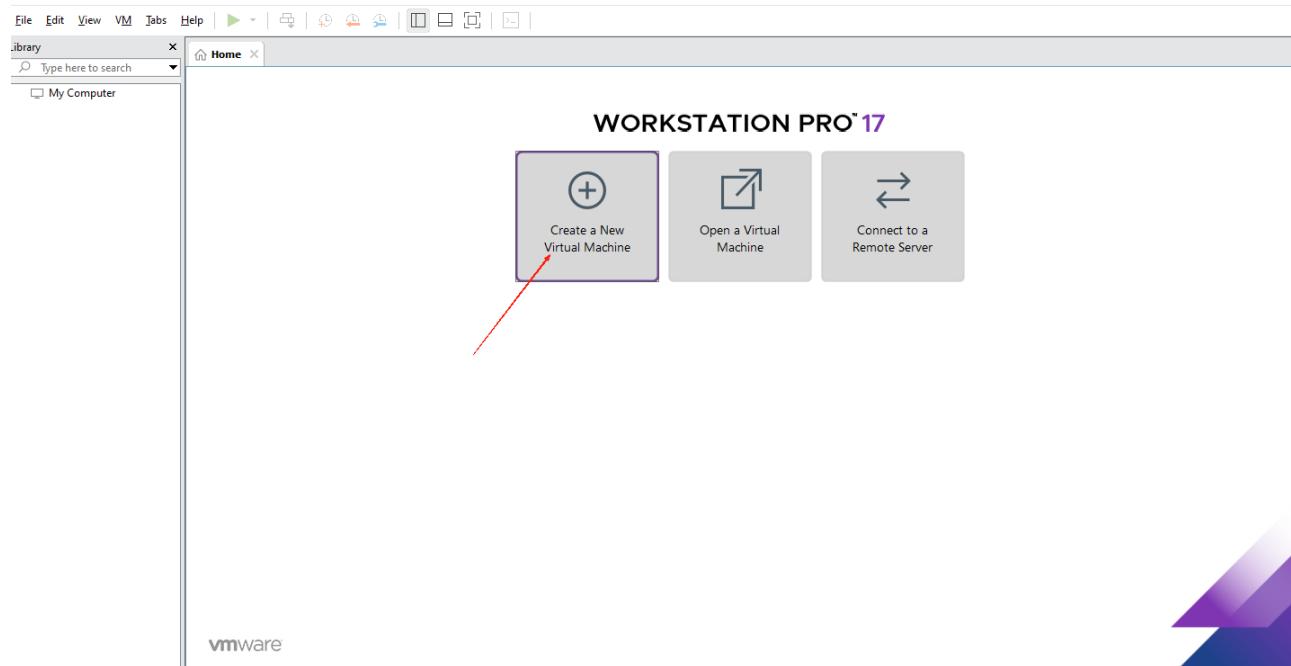
Linux users can skip this step. This section is intended specifically for **Windows users** who need to run a Linux environment using a virtual machine.

You can install a Linux system using either **Windows Subsystem for Linux (WSL)** or a **virtualization tool** such as VMware. In this guide, we demonstrate the setup process using **VMware Workstation**.

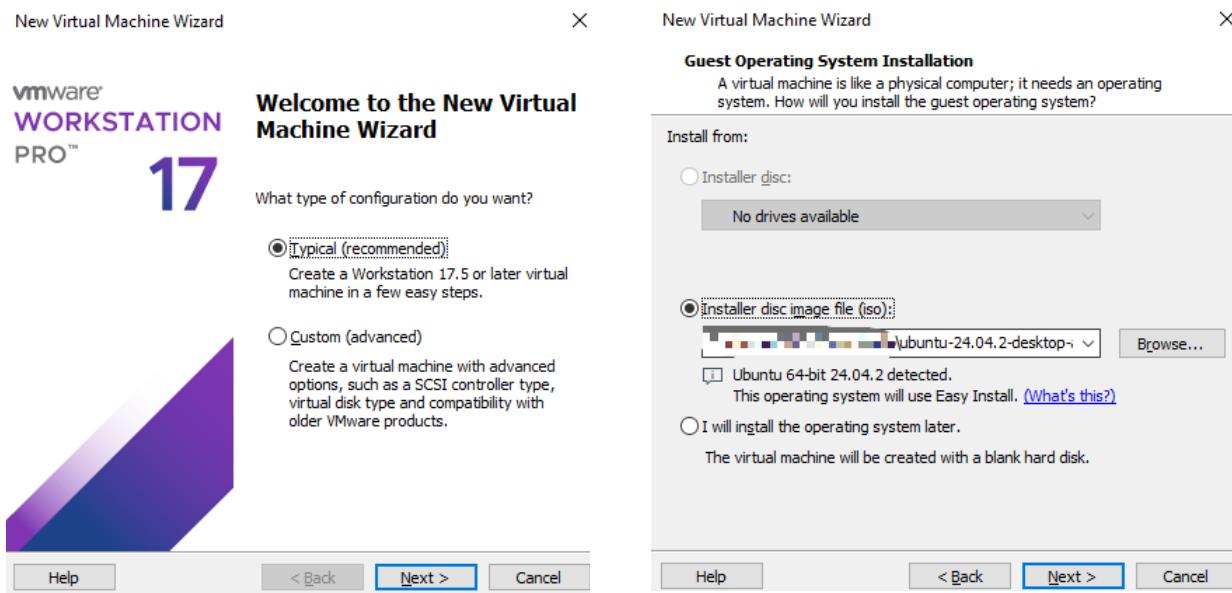
- Download **VMware Workstation/Fusion** from the official VMware website:  
<https://www.vmware.com/products/desktop-hypervisor/workstation-and-fusion>
- Download the **Ubuntu 24.04 Desktop ISO** from:  
<https://ubuntu.com/download/desktop>

Once installed, proceed with the Ubuntu setup and follow the instructions in the subsequent chapters to install the NPB toolkit.

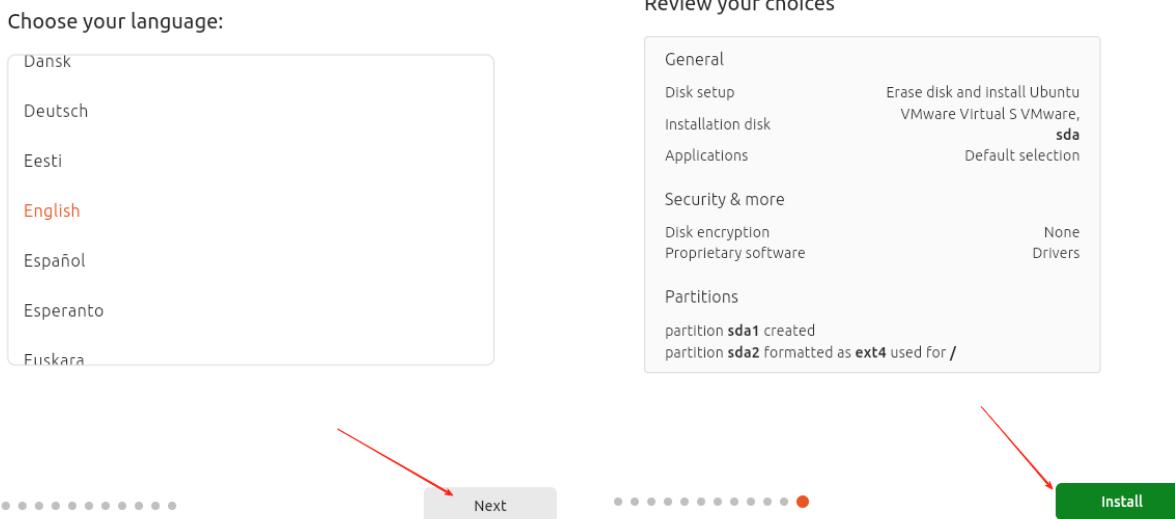
#### Step 1. Create a New Virtual Machine



**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 you encounter any difficulties during the Ubuntu installation, refer to the following video tutorial for detailed, step-by-step guidance:

[https://www.youtube.com/watch?v=SgfrHKg81Qc&ab\\_channel=ProgrammingKnowledge](https://www.youtube.com/watch?v=SgfrHKg81Qc&ab_channel=ProgrammingKnowledge)

Once Ubuntu is installed, continue with the instructions in the following chapters to install and run the NPB toolkit.

## 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>

The screenshot shows the 'Installing Miniconda' page. At the top, there's a link to 'Using Miniconda in a commercial setting?'. Below it, a note says: 'This page contains basic Miniconda installation instructions for Windows, macOS, and Linux, as well as a command-line quickstart installation guide.' A callout box contains the following text: '① 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.' Below this, under 'Basic install instructions', there are links for 'Windows installation' and 'macOS/Linux installation'. Under 'macOS/Linux installation', there are three options: 'macOS graphical installer', 'macOS terminal installer', and 'Linux terminal installer'. A red arrow points from the text 'Linux terminal installer' to the corresponding link. Another red arrow points from the text 'Linux x86' to the 'Linux x86' link in the list below. The list contains: '1. Download the latest version of Miniconda by opening a terminal and running one of the following commands (depending on your Linux architecture):' followed by 'Linux x86' (underlined), 'AWS Graviton2/ARM64', and '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).

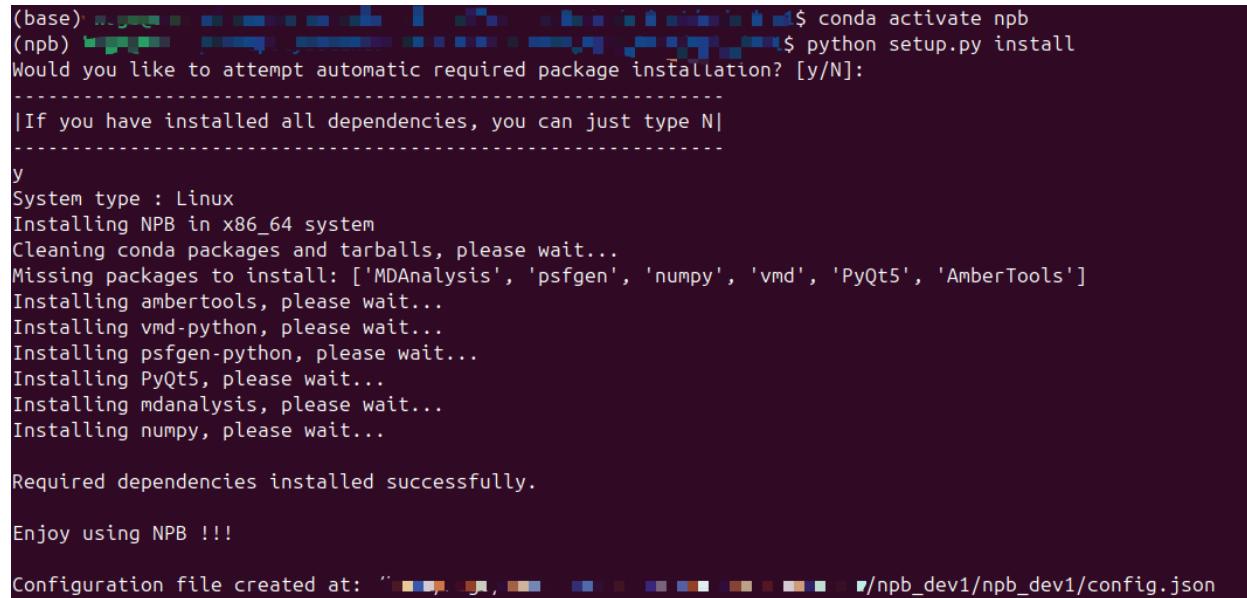
```

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
```

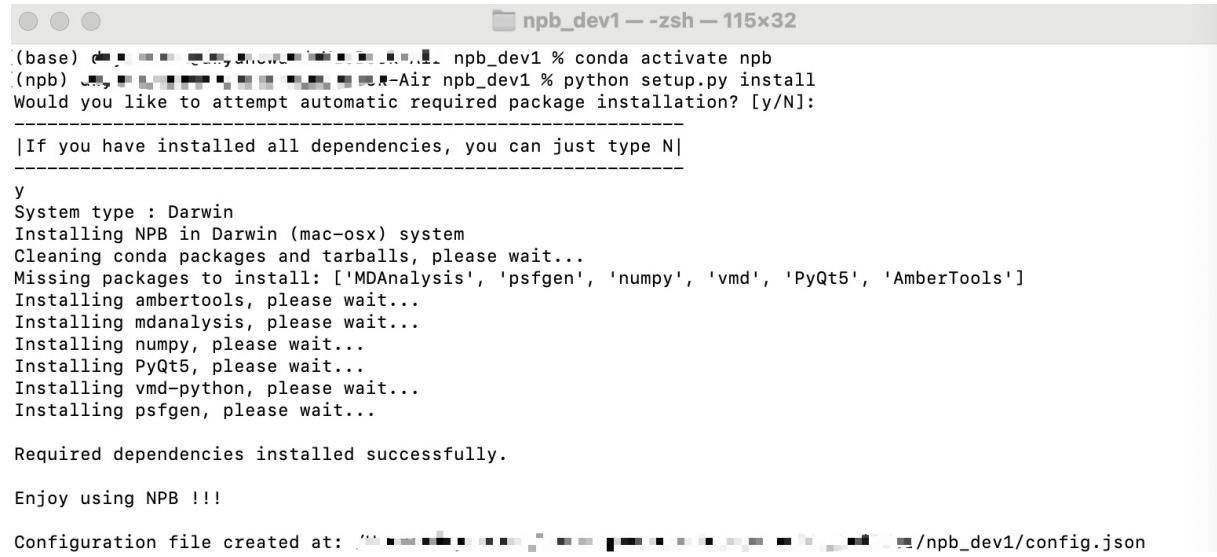
During the installation process, a poor network connection to the Conda servers may cause delays or interruptions in installing dependencies, potentially disrupting the automatic installation (see Figure 2). If this occurs, users can simply re-enter the “**python setup.py install**” command to restart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



```
npb_dev1 -- -zsh -- 115x32
(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 ( $\beta$ -1,4-polyglucans). In addition to higher plants, pure cellulose I $\beta$  is found in certain animal species, such as tunicates, while pure cellulose I $\alpha$  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 $\beta$**  or **Cellulose-I $\alpha$** . 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).

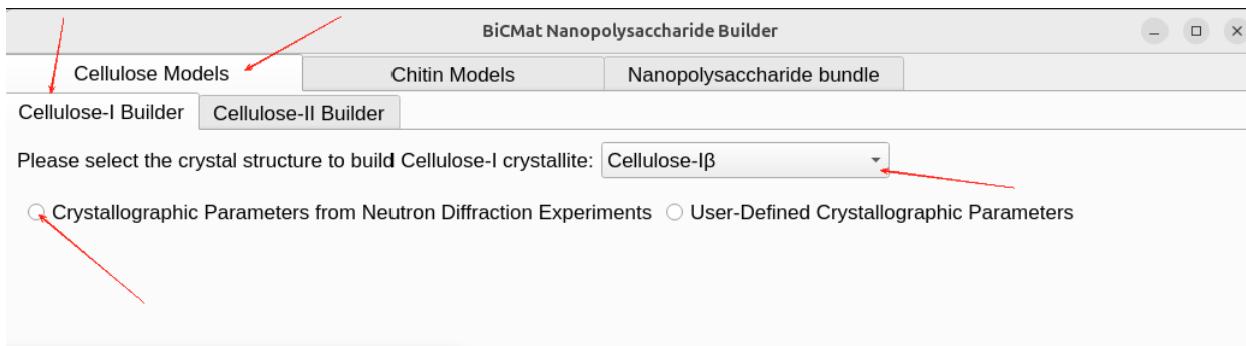


Figure 4

**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 $\beta$

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

18-chain hexagonal cross-section shape

Crystallographic parameters

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

Cross-section width ( $\text{\AA}$ ) Cross-section height ( $\text{\AA}$ )

a repetition b repetition c repetition

Carboxylation  Sulfate  No Modification

a (exp.)=7.784  $\text{\AA}$   
b (exp.)=8.201  $\text{\AA}$   
c (exp.)=10.38  $\text{\AA}$   
 $\gamma$  (exp.)=96.5 $^{\circ}$

II

Cellulose-I $\beta$  unit: Glucose

(110) crystallographic planes

(1-10) crystallographic planes

90 $^{\circ}$

Cross-section of hexagonal-shape Cellulose-I $\beta$  (18-chain model)

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

Cross-section width ( $\text{\AA}$ ) Cross-section height ( $\text{\AA}$ )

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).

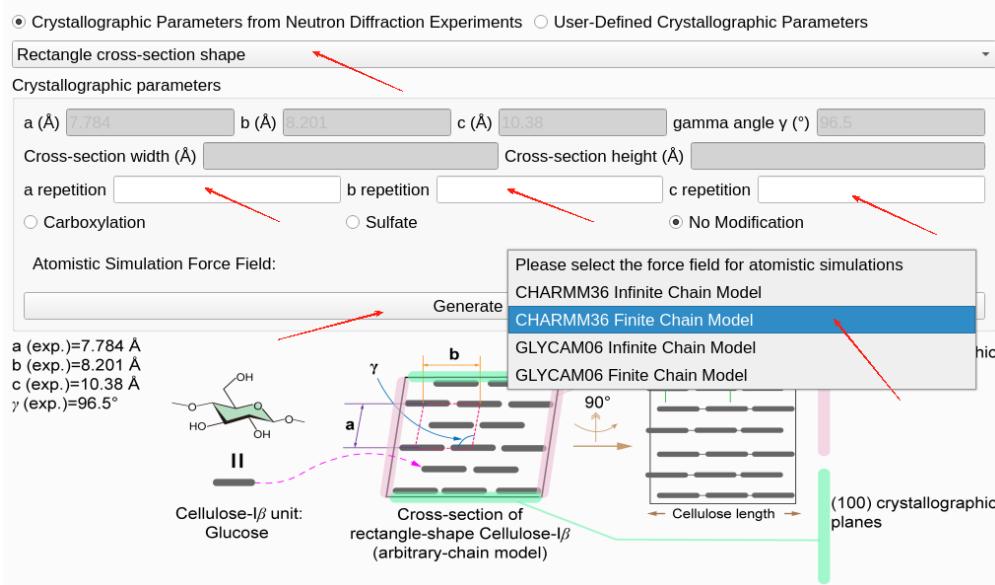


Figure 7

## 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).

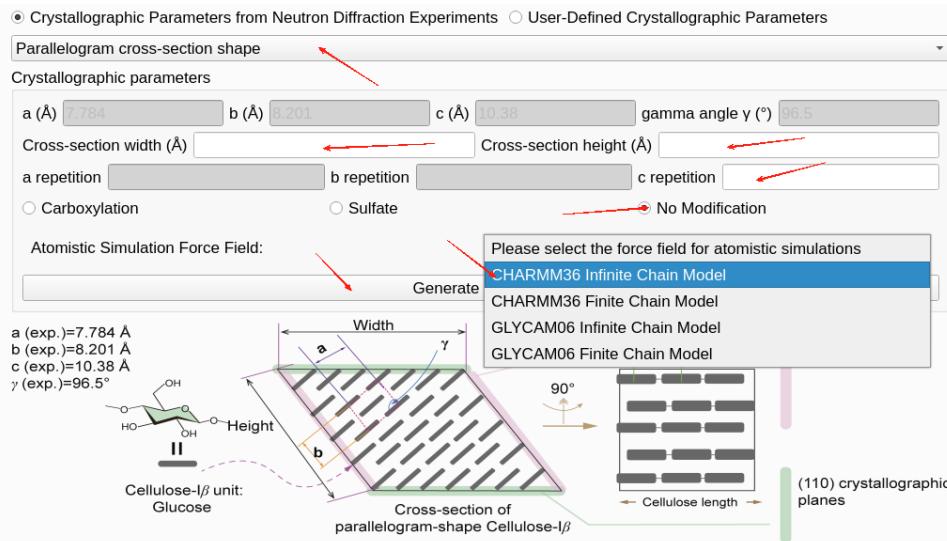


Figure 8

## 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 $\alpha$  and I $\beta$ . **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 $\beta$**

Crystallographic Parameters from Neutron Diffraction Experiments       User-Defined Crystallographic Parameters

18-chain hexagonal cross-section shape

Crystallographic parameters

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

Cross-section width ( $\text{\AA}$ )      Cross-section height ( $\text{\AA}$ )

a repetition      b repetition      c repetition

Carboxylation       Sulfate       No Modification

Please select cellulose-I $\beta$  plane for carboxylation modifications:

Surface charge density (unit: mmol/g):

Atomistic Simulation Force Field:

Generate Structure

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

Figure 9

Please select cellulose-I $\beta$  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**

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

Generate Structure

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  $\alpha$ -chitin nanofibrils often exhibit a hexagonal-shaped cross section. For  $\beta$ -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  $\alpha$ - and  $\beta$ -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 ( $\alpha$ -chitin)

**Step 1.** Select the “Chitin Models” and “ $\alpha$ -chitin Builder” buttons, then use the drop-down menu to choose  $\alpha$ -chitin-A,  $\alpha$ -chitin-B, or  $\alpha$ -chitin-AB. In this context, “-A,” “-B,” and “-AB” indicate that all hydroxymethyl groups at the C<sub>6</sub> 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).

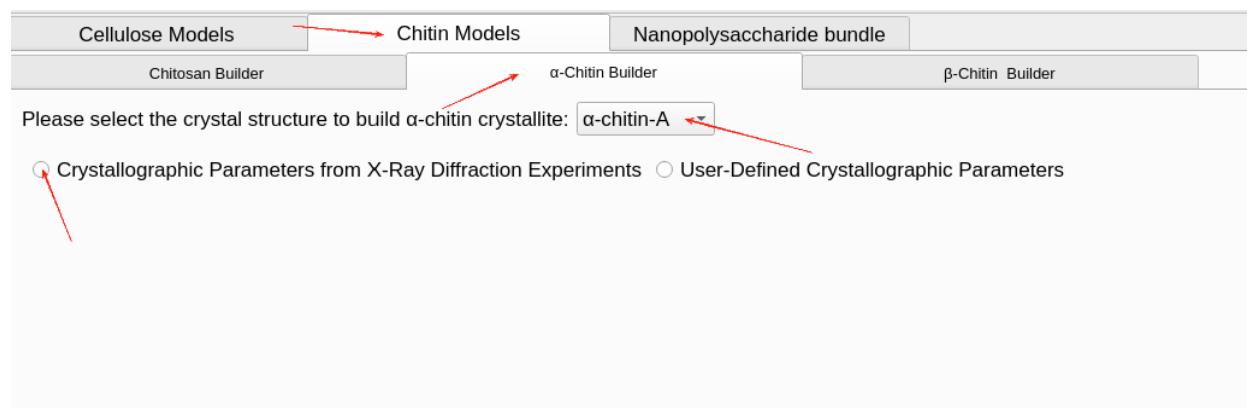
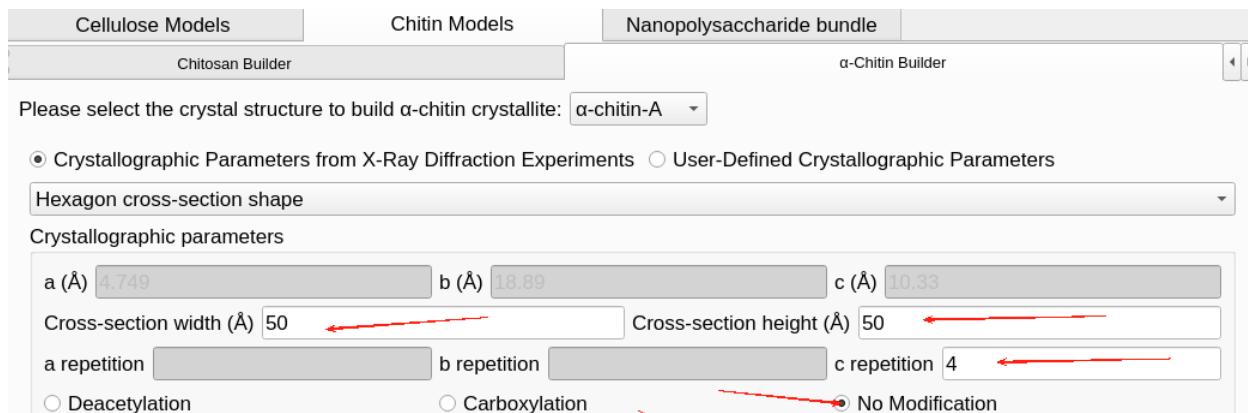


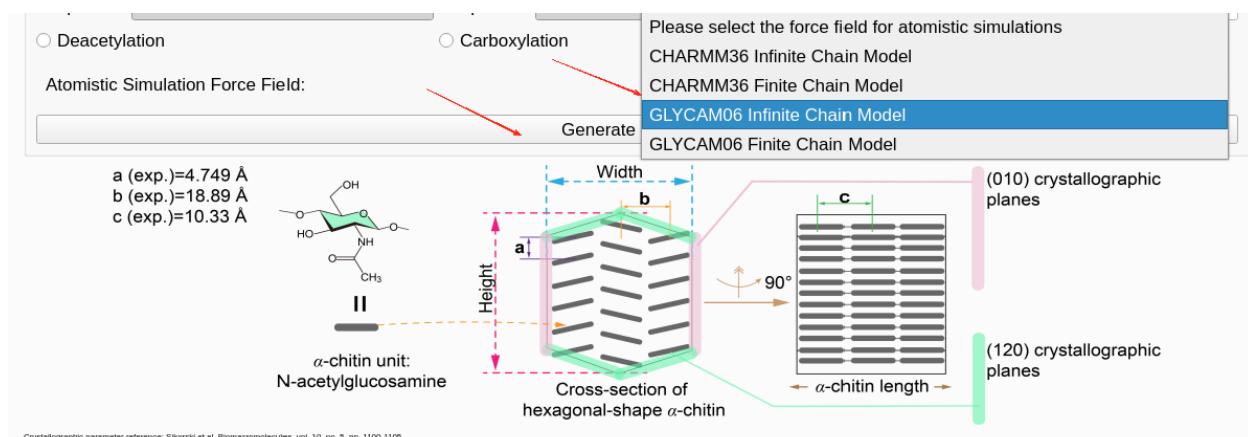
Figure 11

**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**

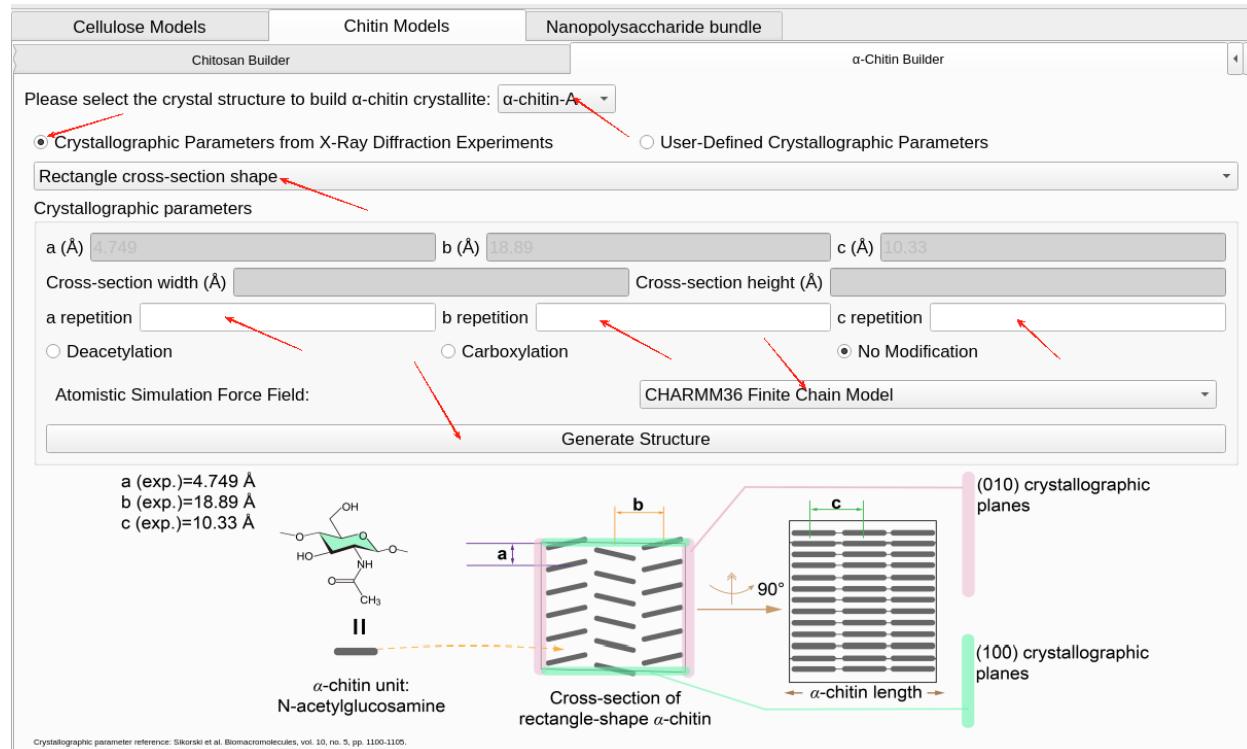
**Step 3.** Use the drop-down menu to select the desired force field. The NPB package currently supports CHARMM36 and GLYCAM06j for  $\alpha$ -chitin native structure. Finally, click the “Generate Structure” button. (Figure 13)



**Figure 13**

### 3.1.b. Rectangle Shape ( $\alpha$ -chitin)

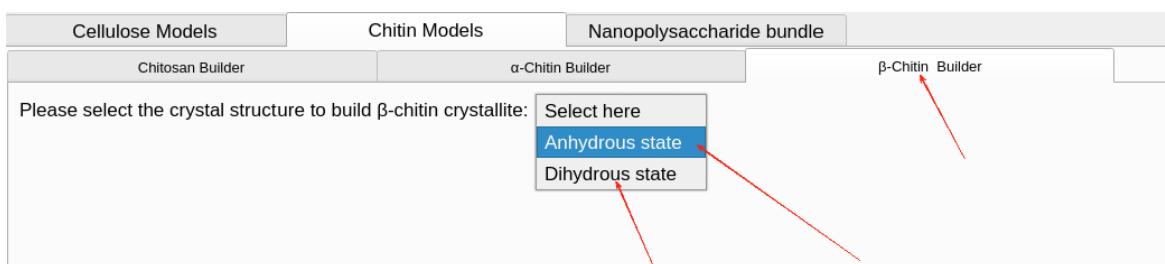
The main steps for building rectangular-shaped chitin are nearly the same as those for the hexagonal cross-section. The only difference is that users must specify the **a**, **b**, and **c** **crystallographic repetitions** and enter them in the appropriate fields (Figure 14). This method can be used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



**Figure 14**

### 3.1.c. Rectangle Shape ( $\beta$ -Chitin: Anhydrous/Dihydrous Configurations)

For  $\beta$ -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).



**Figure 15**

Please select the crystal structure to build  $\beta$ -chitin crystallite: Anhydrous state ▾

Crystallographic Parameters from Neutron Diffraction Experiments  User-Defined Crystallographic Parameters

Rectangle cross-section shape

Crystallographic parameters

a (Å) 4.82	b (Å) 9.24	c (Å) 10.384	gamma angle $\gamma$ (°) 97.16
Cross-section height (010 length) (Å)		Cross-section width (1-20 length) (Å)	
a repetition	b repetition	c repetition	

Deacetylation  Carboxylation  No Modification

Atomistic Simulation Force Field:

Please select the force field for atomistic simulations ▾

Figure 16

### 3.1.d. Parallelogram Shape ( $\beta$ -Chitin: Anhydrous/Dihydrous Configurations)

$\beta$ -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  $\beta$ -chitin, users are referred to this relevant reference (6).

Please select the crystal structure to build  $\beta$ -chitin crystallite: Anhydrous state ▾

Crystallographic Parameters from Neutron Diffraction Experiments  User-Defined Crystallographic Parameters

Parallelogram cross-section shape

Crystallographic parameters

a (Å) 4.82	b (Å) 9.24	c (Å) 10.384	gamma angle $\gamma$ (°) 97.16
Cross-section height (010 length) (Å)		Cross-section width (1-20 length) (Å)	
a repetition	b repetition	c repetition	

Deacetylation  Carboxylation  No Modification

Atomistic Simulation Force Field:

Please select the force field for atomistic simulations ▾

$a$  (exp.)=4.819 Å  
 $b$  (exp.)=9.239 Å  
 $c$  (exp.)=10.38 Å  
 $\gamma$  (exp.)=97.16°

**II**  
 **$\beta$ -chitin unit: N-acetylglucosamine**

**Cross-section of parallelogram-shape  $\beta$ -chitin**  
**(010) crystallographic planes**  
**(1-20) crystallographic planes**  
 **$\beta$ -chitin length**

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  $\alpha$ - and  $\beta$ -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  $\alpha$ -chitin crystallite:

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

Rectangle cross-section shape

Crystallographic parameters

a (Å) <input type="text" value="4.749"/>	b (Å) <input type="text" value="18.89"/>	c (Å) <input type="text" value="10.33"/>
Cross-section width (Å) <input type="text"/>		Cross-section height (Å) <input type="text"/>
a repetition <input type="text"/>	b repetition <input type="text"/>	c repetition <input type="text"/>

Deacetylation       Carboxylation       No Modification

Please select  $\alpha$ -chitin plane for deacetylation modifications:

Degree of deacetylation ( $\geq 0$  and  $< 1$ ):

Atomistic Simulation Force Field:

a (exp.)=4.749 Å  
b (exp.)=18.89 Å  
c (exp.)=10.33 Å

II

α-chitin unit:  
N-acetylglucosamine

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

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  $\alpha$ -chitin

(100) crystallographic planes

α-chitin length

Figure 18

Deacetylation       Carboxylation       No Modification

Please select  $\alpha$ -chitin plane for deacetylation modifications:

Degree of deacetylation ( $\geq 0$  and  $< 1$ ):

Atomistic Simulation Force Field:

pH level of  $\alpha$ -chitin structure ( $> 0$  and  $< 14$ ):

Generate Structure

Figure 19

#### 4. Construction of Nanopolysaccharide Bundles

NPB currently supports the construction of **cellulose I $\beta$  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 nanopolsaccharides—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 1 C1 4GB 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 2 H1 4GB 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 3 O5 4GB 1 12.153 11.223 0.242 1.00 0.00 O
ATOM 4 H5 BGLC 1 10.985 11.749 1.761 1.00 0.00 H	ATOM 4 C5 4GB 1 10.889 11.258 0.920 1.00 0.00 C
ATOM 5 O5 BGLC 1 12.153 11.223 0.242 1.00 0.00 O	ATOM 5 H5 4GB 1 10.985 11.749 1.761 1.00 0.00 H
ATOM 6 C2 BGLC 1 11.723 13.135 -1.146 1.00 0.00 C	ATOM 6 C6 4GB 1 10.518 9.820 1.214 1.00 0.00 C
ATOM 7 H2 BGLC 1 11.623 12.562 -1.934 1.00 0.00 H	ATOM 7 H61 4GB 1 10.256 9.375 0.395 1.00 0.00 H
ATOM 8 O2 BGLC 1 12.278 14.398 -1.514 1.00 0.00 O	ATOM 8 H62 4GB 1 11.293 9.354 1.573 1.00 0.00 H
ATOM 9 H02 BGLC 1 13.198 14.271 -1.209 1.00 0.00 H	ATOM 9 O6 4GB 1 9.460 9.754 2.150 1.00 0.00 O
ATOM 10 C3 BGLC 1 10.386 13.310 -0.452 1.00 0.00 C	ATOM 10 H60 4GB 1 9.768 8.997 2.681 1.00 0.00 H
ATOM 11 H3 BGLC 1 10.500 13.911 0.312 1.00 0.00 H	ATOM 11 C4 4GB 1 9.873 11.962 0.042 1.00 0.00 C
ATOM 12 O3 BGLC 1 9.469 13.893 -1.372 1.00 0.00 O	ATOM 12 H4 4GB 1 9.677 11.398 -0.733 1.00 0.00 H
ATOM 13 H03 BGLC 1 8.718 14.066 -0.778 1.00 0.00 H	ATOM 13 C3 4GB 1 10.386 13.310 -0.452 1.00 0.00 C
ATOM 14 C4 BGLC 1 9.873 11.962 0.042 1.00 0.00 C	ATOM 14 H3 4GB 1 10.500 13.911 0.312 1.00 0.00 H
ATOM 15 H4 BGLC 1 9.677 11.398 -0.733 1.00 0.00 H	ATOM 15 O3 4GB 1 9.469 13.893 -1.372 1.00 0.00 O
ATOM 16 O4 BGLC 1 8.676 12.109 0.825 1.00 0.00 O	ATOM 16 H30 4GB 1 8.718 14.066 -0.778 1.00 0.00 H
ATOM 17 C6 BGLC 1 10.518 9.820 1.214 1.00 0.00 C	ATOM 17 C2 4GB 1 11.723 13.135 -1.146 1.00 0.00 C
ATOM 18 H61 BGLC 1 10.256 9.375 0.395 1.00 0.00 H	ATOM 18 H2 4GB 1 11.623 12.562 -1.934 1.00 0.00 H
ATOM 19 H62 BGLC 1 11.293 9.354 1.573 1.00 0.00 H	ATOM 19 O2 4GB 1 12.278 14.398 -1.514 1.00 0.00 O
ATOM 20 O6 BGLC 1 9.468 9.754 2.150 1.00 0.00 O	ATOM 20 H20 4GB 1 13.198 14.271 -1.209 1.00 0.00 H
ATOM 21 H06 BGLC 1 9.768 8.997 2.681 1.00 0.00 H	ATOM 21 O4 4GB 1 8.676 12.109 0.825 1.00 0.00 O
ATOM 22 C1 BGLC 2 7.472 11.860 0.163 1.00 0.00 C	ATOM 22 C1 4GB 2 7.472 11.860 0.163 1.00 0.00 C
ATOM 23 H1 BGLC 2 7.583 11.251 -0.599 1.00 0.00 H	ATOM 23 H1 4GB 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 24 O5 4GB 2 6.946 13.131 -0.231 1.00 0.00 O
ATOM 25 H5 BGLC 2 5.793 12.557 -1.752 1.00 0.00 H	ATOM 25 C5 4GB 2 5.689 13.071 -0.920 1.00 0.00 C
ATOM 26 O5 BGLC 2 6.946 13.131 -0.231 1.00 0.00 O	ATOM 26 H5 4GB 2 5.793 12.557 -1.752 1.00 0.00 H
ATOM 27 C2 BGLC 2 6.518 11.277 1.230 1.00 0.00 C	ATOM 27 C6 4GB 2 5.338 14.522 -1.241 1.00 0.00 C
ATOM 28 H2 BGLC 2 6.461 11.886 1.993 1.00 0.00 H	ATOM 28 H61 4GB 2 5.068 14.979 -0.428 1.00 0.00 H
ATOM 29 O2 BGLC 2 7.056 10.023 1.645 1.00 0.00 O	ATOM 29 H62 4GB 2 6.100 14.978 -1.615 1.00 0.00 H
ATOM 30 H02 BGLC 2 7.867 10.311 2.103 1.00 0.00 H	ATOM 30 O6 4GB 2 4.265 14.539 -2.171 1.00 0.00 O
ATOM 31 C3 BGLC 2 5.164 11.112 0.599 1.00 0.00 C	ATOM 31 H60 4GB 2 4.717 14.928 -2.938 1.00 0.00 H
ATOM 32 H3 BGLC 2 5.219 10.458 -0.106 1.00 0.00 H	ATOM 32 C4 4GB 2 4.675 12.488 -0.816 1.00 0.00 C
ATOM 33 O3 BGLC 2 4.266 10.653 1.614 1.00 0.00 O	ATOM 33 H4 4GB 2 4.469 13.028 0.714 1.00 0.00 H
ATOM 34 H03 BGLC 2 3.418 11.002 1.235 1.00 0.00 H	ATOM 34 C3 4GB 2 5.164 11.112 0.599 1.00 0.00 C
ATOM 35 C4 BGLC 2 4.675 12.409 -0.016 1.00 0.00 C	ATOM 35 H3 4GB 2 5.219 10.430 -0.186 1.00 0.00 H
ATOM 36 H4 BGLC 2 4.469 13.028 0.714 1.00 0.00 H	ATOM 36 O3 4GB 2 4.266 10.653 1.614 1.00 0.00 O
ATOM 37 O4 BGLC 2 3.488 12.243 -0.799 1.00 0.00 O	ATOM 37 H30 4GB 2 3.418 11.002 1.235 1.00 0.00 H
ATOM 38 C6 BGLC 2 5.338 14.522 -1.241 1.00 0.00 C	ATOM 38 C2 4GB 2 6.518 11.277 1.230 1.00 0.00 C
ATOM 39 H61 BGLC 2 5.068 14.979 -0.428 1.00 0.00 H	ATOM 39 H2 4GB 2 6.461 11.886 1.993 1.00 0.00 H
ATOM 40 H62 BGLC 2 6.100 14.978 -1.615 1.00 0.00 H	ATOM 40 O2 4GB 2 7.056 10.023 1.645 1.00 0.00 O
ATOM 41 O6 BGLC 2 4.265 14.539 -2.171 1.00 0.00 O	ATOM 41 H20 4GB 2 7.867 10.311 2.103 1.00 0.00 H
ATOM 42 H06 BGLC 2 4.717 14.928 -2.938 1.00 0.00 H	ATOM 42 O4 4GB 2 3.488 12.423 -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 <sup>th</sup> Column Variable Name (in PDB file)	5 <sup>th</sup> Column Variable Name (in PDB file)
Cellulose I $\alpha$	CHARMM36	chain_ud.pdb	BGLC	1, 2
Cellulose I $\alpha$ (Finite model)	GLYCAM06j	chain-finite_ud.pdb	4GB	2, 3
Cellulose I $\alpha$ (Infinite model)	GLYCAM06j	chain_ud.pdb	4GB	1, 2
Cellulose I $\beta$	CHARMM36	chain-1_ud.pdb chain-2_ud.pdb	BGLC	1, 2
Cellulose I $\beta$ (Finite model)	GLYCAM06j	chain-1-finite_ud.pdb chain-2-finite_ud.pdb	4GB	2, 3
Cellulose I $\beta$ (Infinite model)	GLYCAM06j	chain-1_ud.pdb chain-2_ud.pdb	4GB	1, 2
$\alpha$ -chitin	CHARMM36	left-unit_ud.pdb right-unit_ud.pdb	BLNAN	1, 2
$\alpha$ -chitin (Finite model)	GLYCAM06j	left-unit-finite_ud.pdb right-unit-finite_ud.pdb	4YB	2, 3
$\alpha$ -chitin (Infinite model)	GLYCAM06j	left-unit_ud.pdb right-unit_ud.pdb	4YB	1, 2
$\beta$ -chitin (Anhydrous)	CHARMM36	unit-ud.pdb	BLNA	1, 2
$\beta$ -chitin (Dihydrous)	CHARMM36	dihydrous-unit-ud.pdb	BDNA	1, 2
$\beta$ -chitin (Anhydrous; Finite)	GLYCAM06j	unit-ud-finite.pdb	4YB	2, 3
$\beta$ -chitin (Anhydrous; Infinite)	GLYCAM06j	unit-ud.pdb	4YB	1, 2

**Note:** For cellulose I $\alpha$ , 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 $\beta$  and  $\alpha$ -chitin, users must provide two chain units. Additional information can be found in the ./npb\_dev1/structure directory.

For  $\beta$ -chitin, NPB currently supports both anhydrous and dihydrous configurations in the CHARMM36 format. Users should note that the dihydrous 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  $\beta$ -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 5<sup>th</sup> 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.

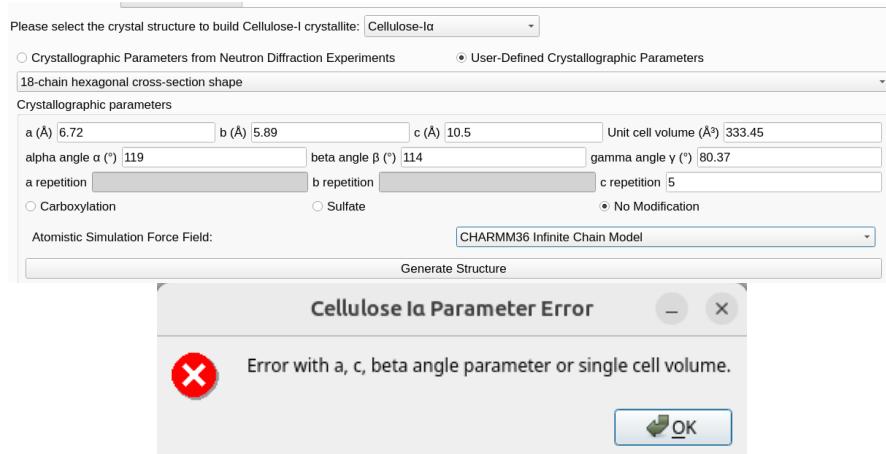
For the **GLYCAM06j** force field, the structure includes a reducing end (ROH) to construct a **finite-length nanopolysaccharide**. When preparing the two-sugar units for GLYCAM06j, users should **start the resid numbering from 2 to 3(the 5th column number in the PDB file)**. Additionally, the file should 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-Iα 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- $\text{\textit{I}\alpha}$

In this example, we used NPB to produce a cellulose- $\text{\textit{I}\alpha}$  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 min300.mdcrd
08
09 /path/to/AMBER/pmemd.cuda -O -i pr.mdin -o pr.out -p cell_solv.prmtop -c min300.rst -r
10 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- $\text{I}\beta$ bundle

In this example, we used NPB to generate a cellulose- $\text{I}\beta$  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
```

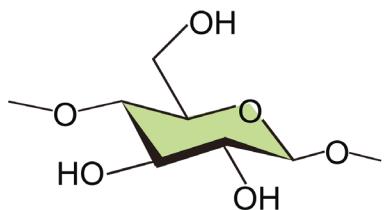
If users wish to perform the simulation in the hydrated state, one additional step is required before running the GROMACS “`grompp`” script mentioned above. A TIP3P-Charmm compatible “`.itp`” file is also provided in the `gmx` folder.

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

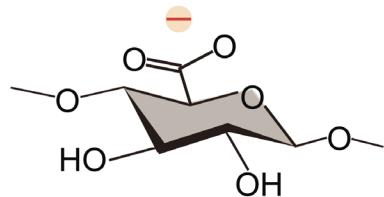
## 7. Monosaccharide Topologies Utilized in NPB

### 7.1. CHARMM36 Force Field

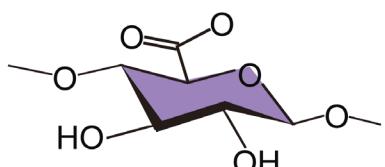
#### 7.1.a Cellulose



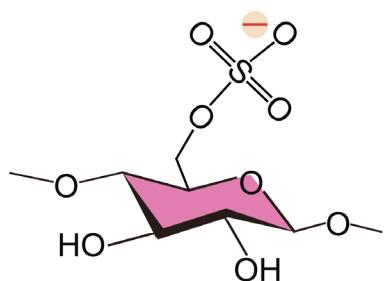
Glucose  
Resname : BGLC



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)**

<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
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

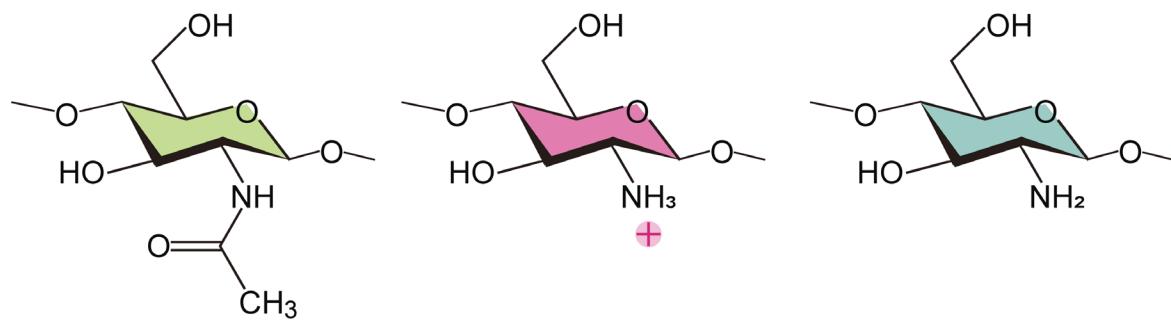
**Table 4.**  
**Atom list of resname BG LD (structure with a net charge of 0)**

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)**

<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
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		

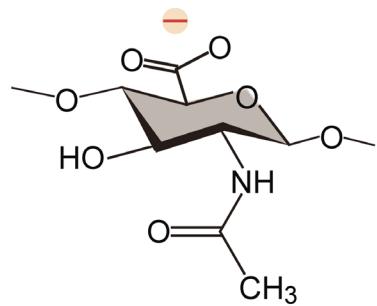
### 7.1.b Chitin



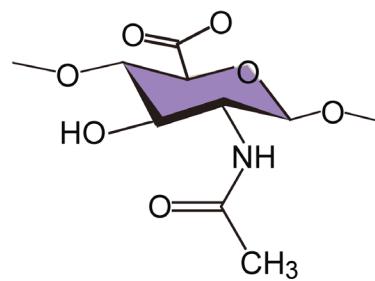
N-Acetylglucosamine  
Resname : BLNA

Protonated Glucosamine  
Resname : BLNP

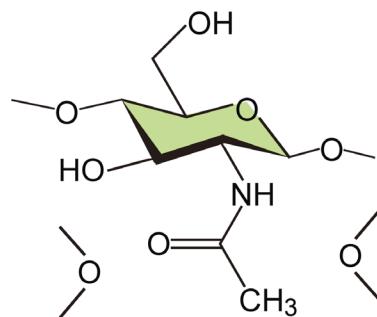
Deprotonated Glucosamine  
Resname : BLND



Deprotonated N-acetylglucosaminuronic Acid  
Resname : BLCP



Protonated N-acetylglucosaminuronic Acid  
Resname : BLCD



Dihydros 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)**

<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
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)**

<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
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)**

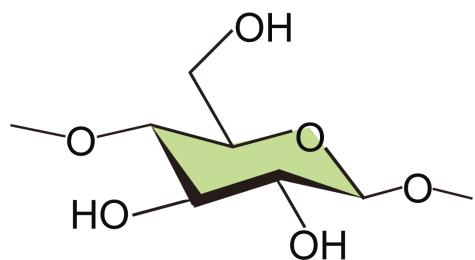
<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
C1	CC3162	C2	CC3161
H1	HCA1	H2	HCA1
O1 (Reduced end)	OC311	N	NC2D1
HO1 (Reduced end)	HCP1	HN	HCP1
C5	CC3163	C	CC201
H5	HCA1	O	OC2D1
O5	OC3C61	CT	CC331
C4	CC3161	HT1	HCA3
H4	HCA1	HT2	HCA3
O4	OC311	HT3	HCA3
HO4 (Non-reduced end)	HCP1	C3	CC3161
C6	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)**

<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
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

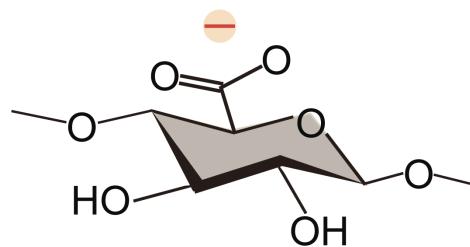
## 7.2. GLYCAM06j Force Field

### 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.

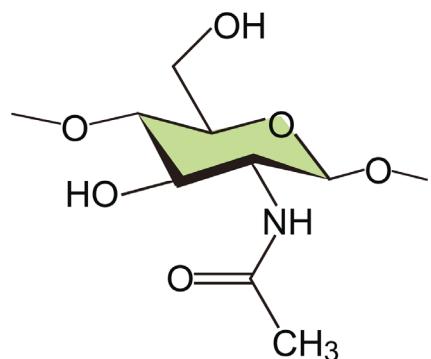
**Table 12.**  
**Atom list of resname 4GB/0GB (structure with a net charge of 0)**

<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
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)**

<b>Atom</b>	<b>Atomtypes</b>	<b>Atom</b>	<b>Atomtypes</b>
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 GLYCAMS06j force field.

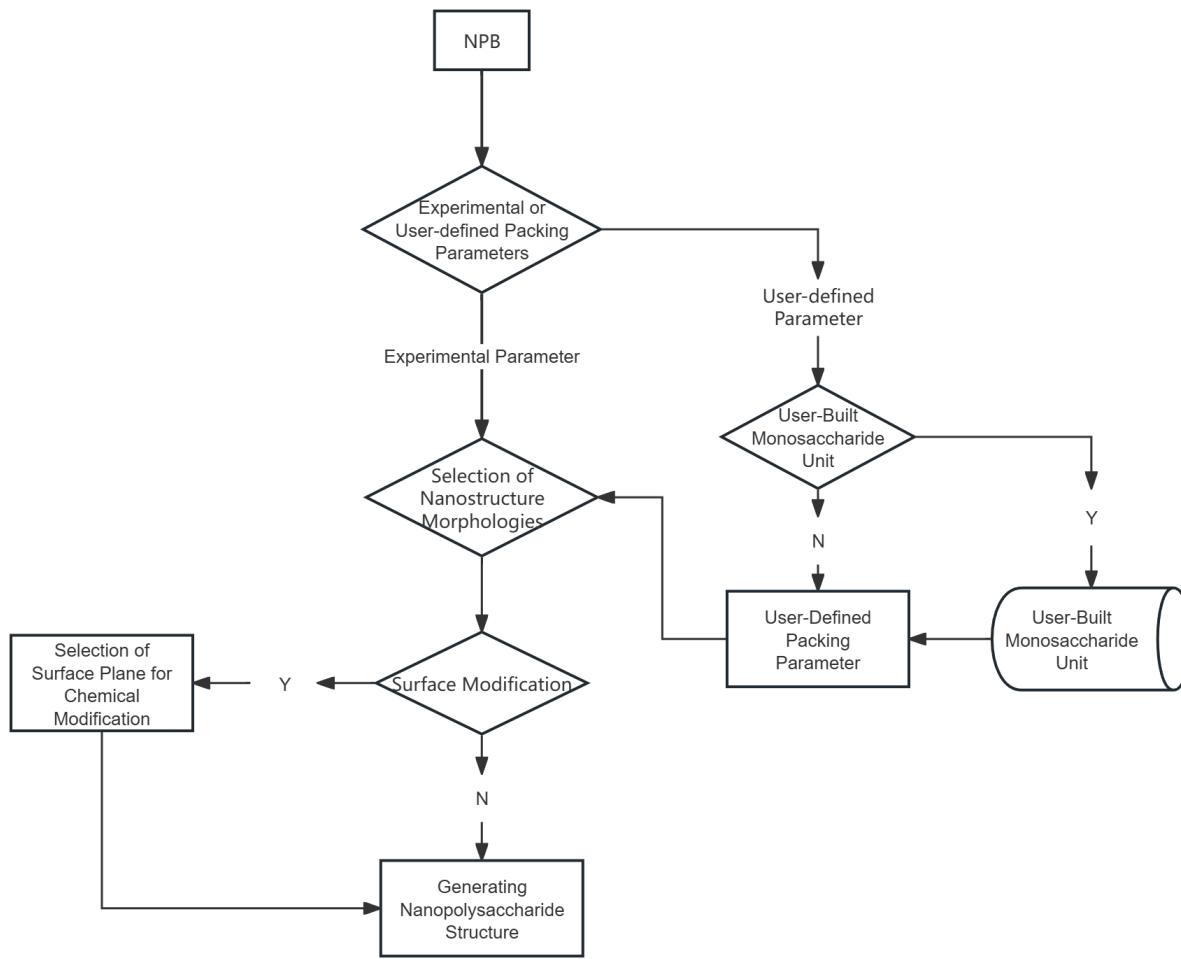
**Table 14.**  
**Atom list of resname 4YB/0YB (structure with a net charge of 0)**

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.



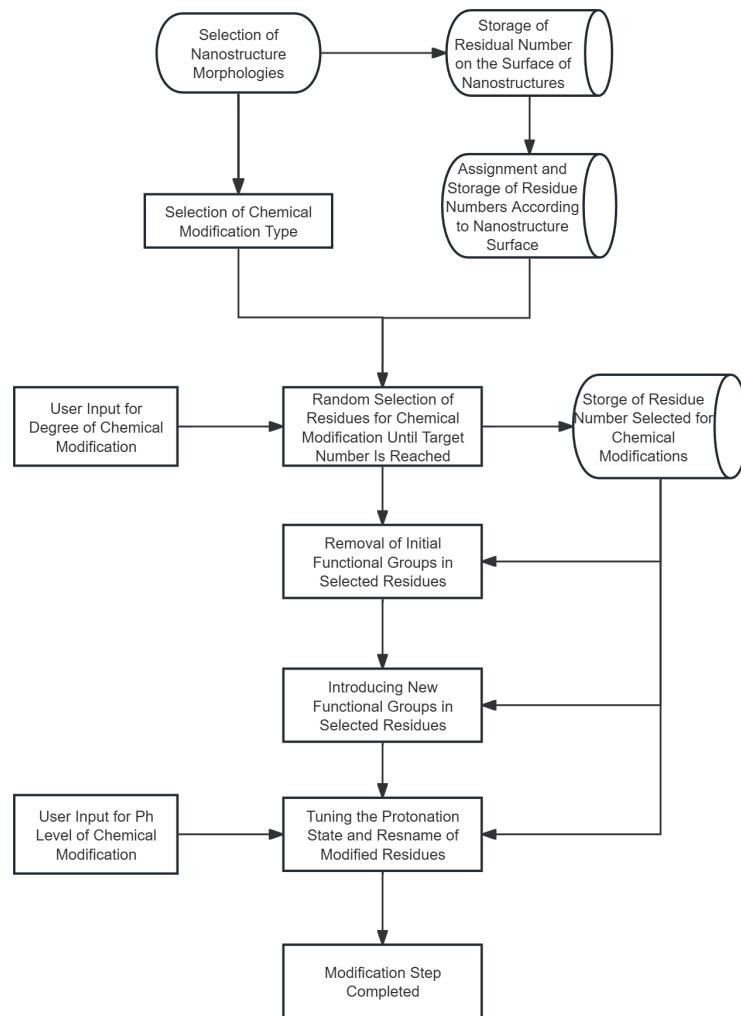
**Figure 28.** Flowchart of the detailed procedure for building nanopolysaccharide structures with the NPB package.

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 specific chains at the surface are selected to be substituted 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

## **9. Update logs**

Dev\_1.1.0 – Added support for building mercerized cellulose II structures and generating corresponding topology files.

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