winmostar tutorial

Gromacs Protein

V11.3.1

21 Oct. 2022 X-Ability Co., Ltd.

About This Manual

- This manual is a tutorial demonstrating use cases for Winmostar V11.
- For those using Winmostar V11 for the first time, please consult Beginner's Guide.
- For those who wish to explore the details of each feature, please refer to Winmostar User Manual.
- Those who wish to practice the contents of this manual are encouraged to attend a training session.
  - Winmostar Introductory Training Session:This guide only introduces the operation methods of the Basic Tutorial.
  - Winmostar Basic Training Session:We will cover the theoretical background, explanations on interpreting results, operational methods of the Basic Tutorial, and procedures for some tutorials beyond the basic level.
  - Individual Training Session:You can freely customize the training content according to your preferences.
- If you are unable to proceed with the operations as outlined in this manual, please first consult Frequently asked questions.
- If your issue is not resolved through the Frequently Asked Questions, for the purpose of information accumulation and management, please contact us using Contact page. Attach files generated at the time of the issue and provide steps to reproduce the problem.
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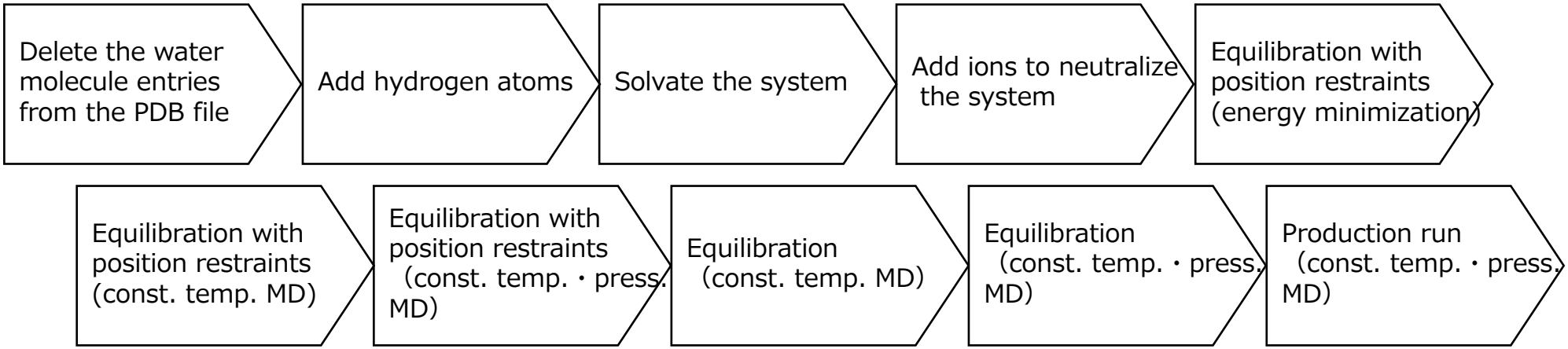
Overview

- This tutorial explains how to prepare a Gromacs input from the PDB file of chicken egg-white lysozyme, enabling molecular dynamics simulations.



Note :

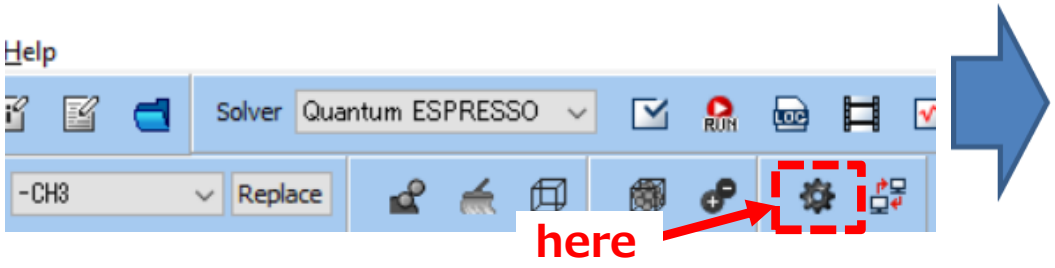
- Crystal water from the XRD-derived PDB file should be removed, and missing hydrogen atoms must be added.
- The system size, such as the number of solvent molecules, can significantly affect protein behavior.
- The required number of equilibration steps may vary depending on molecular species and initial density.
- Calculation results are also strongly influenced by the chosen force field and interaction methods.

Operating Environment Settings

- To use this feature, it is necessary to set up Cygwin.
- https://winmostar.com/en/installation/ Set up Cygwin by following the configuration steps outlined in the installation instructions.

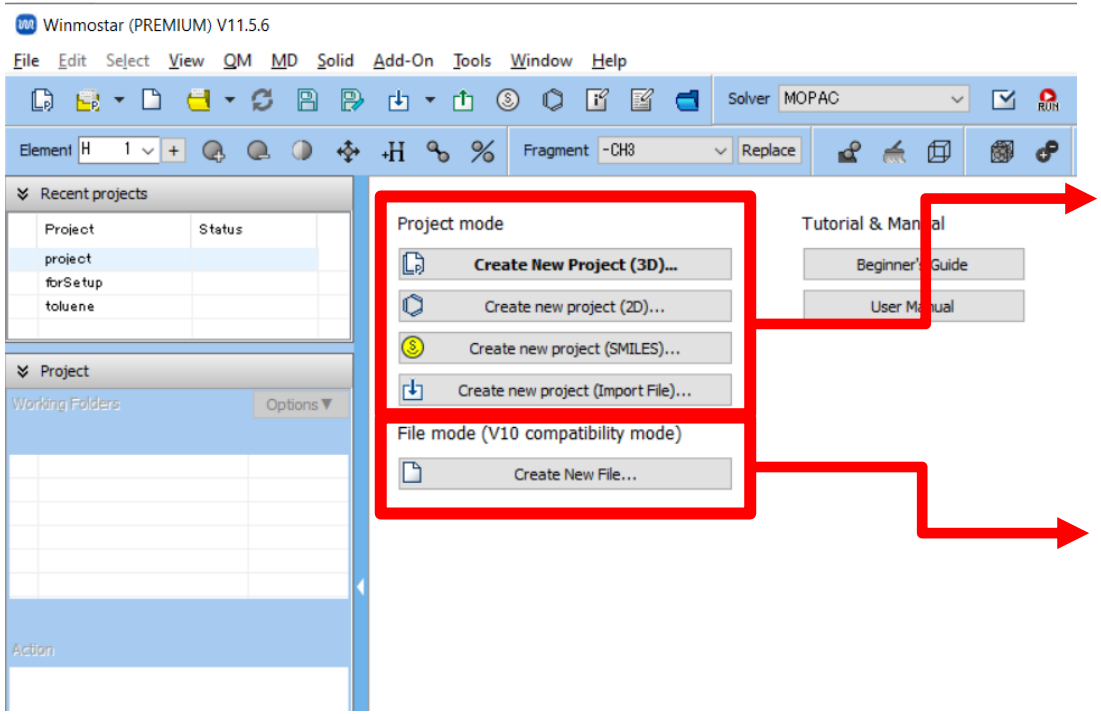
(7) Install Cygwin environment for Winmostar. ← here

- By default, it is installed directly under C:, but you can install it in a location of your choice by changing the 'Program Path' > 'Cygwin' in Winmostar Preference.



Operating Modes of Winmostar V11

V11 offers two operating modes: **Project Mode** and **File Mode**.
This manual focuses on operations in Project Mode.
For operations in File Mode, please refer to LAMMPS Tutorial for V10.



Project Mode New Features in V11

Users can manage jobs without having to manage individual files.
We generally recommend using this mode.

File Mode

Users explicitly create and manage individual files.
The operational procedure is the same as from V10 and earlier versions.

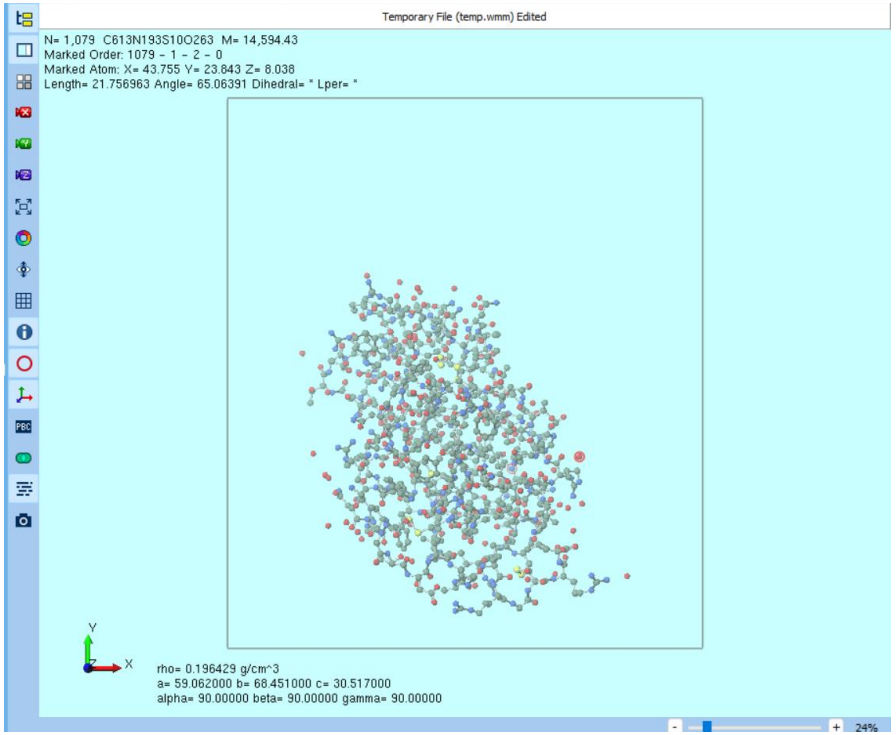
A. Modeling of the System

For basic operations, please refer to Gromacs Basics tutorial.

A. Click **File | New Project**, enter '`protein`' in **Project name**, and click **Save**.

B. Click **File | Import | Sample File | 1aki.pdb.**
   - If you wish to load a different file at this stage, use **File | Import File** instead.

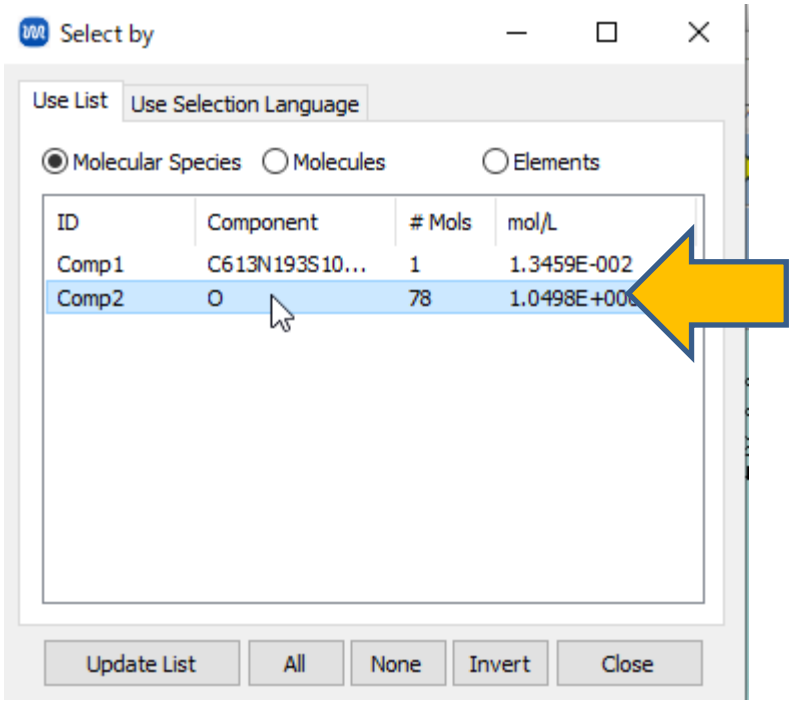
C. In **Import File** dialog, click **Discard and import**.

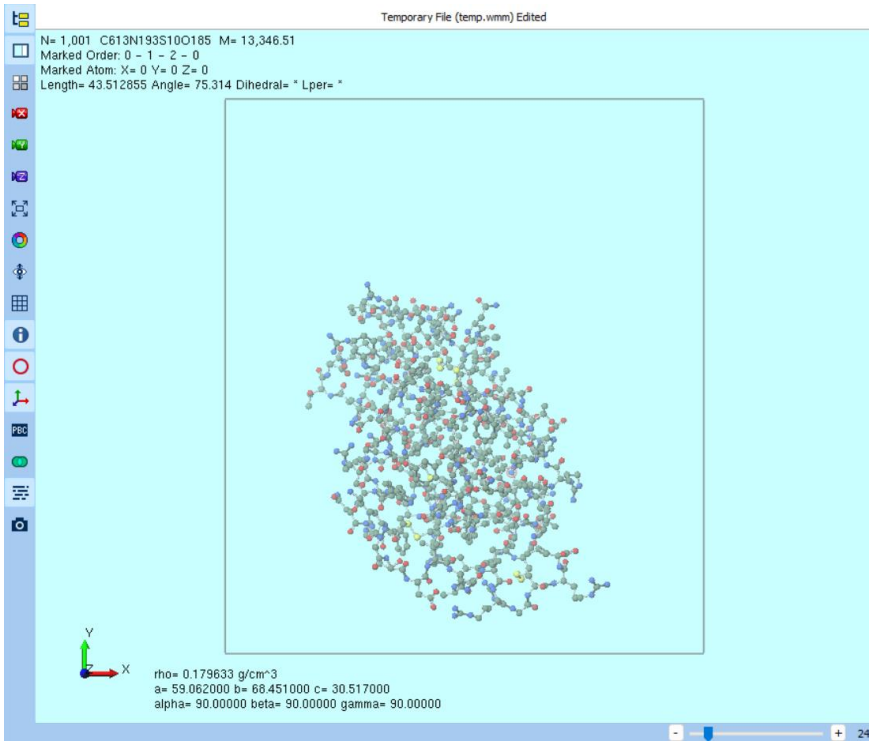


A. Modeling of the System

A. Click **Select | Select by Molecular Species**, click on the row for **Comp2 O 78**, and then click **Close**.

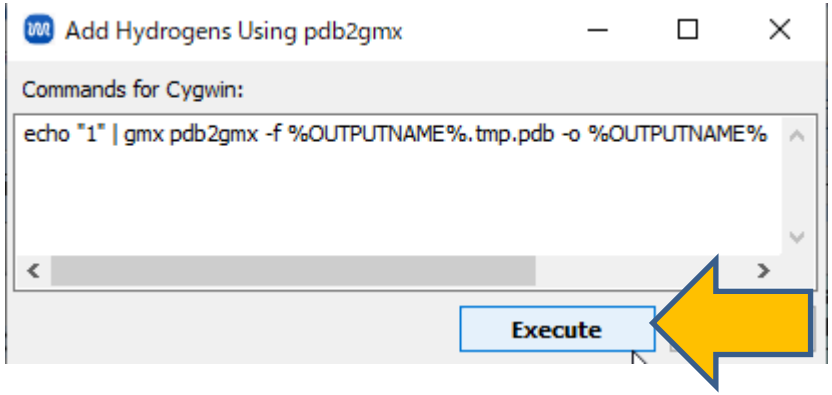
B. Click  **(Modify Selected Group) | Delete**, and when asked 'Do you want to delete or leave group?' click **Delete**.

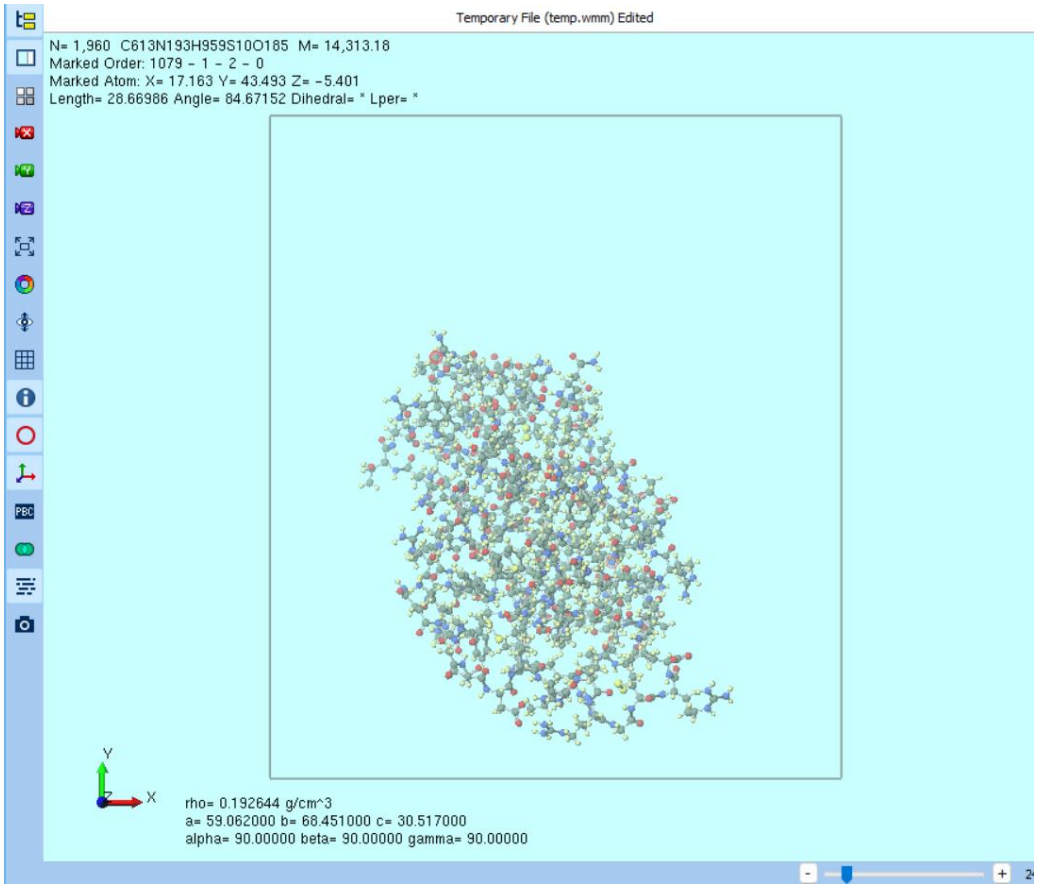




A. Modeling of the System

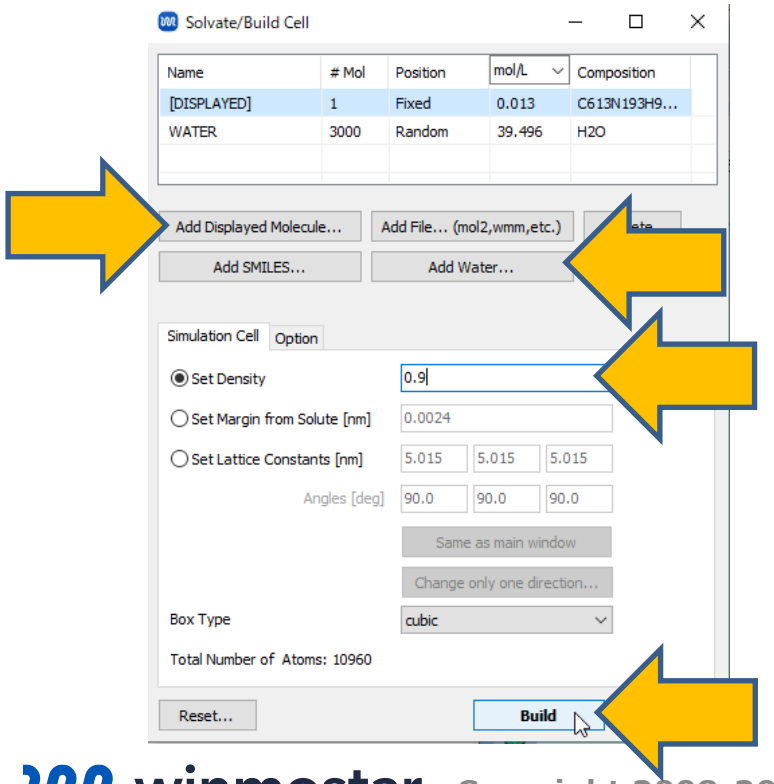
A. Click **Edit | Add Hydrogens | Using pdb2gmx…** and then **Execute.**
- Even if the PDB file already includes hydrogen atoms, this step may still be necessary to ensure proper force field assignment based on residue information later.

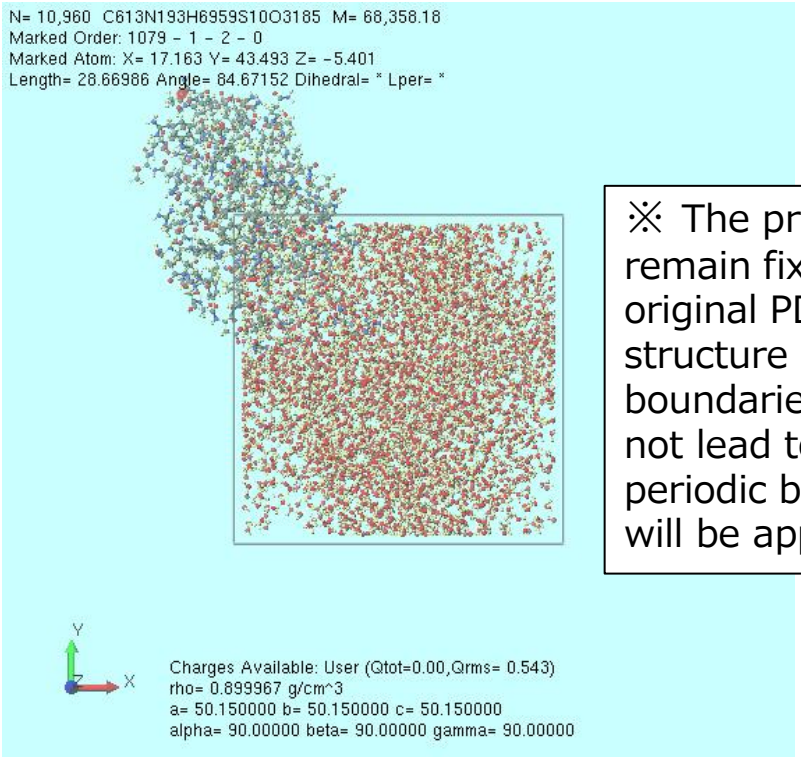




A. Modeling of the System

A. Click **Solvate/Build Cell**.
B. Click **Add Displayed Molecule**, enter '**1**', and click **OK**.
C. Click **Add Water**, enter '3000', and click **OK**.
D. Enter '0.9' in **Set Density** and click **Build** and when asked '…you want to continue?' click **Yes**.

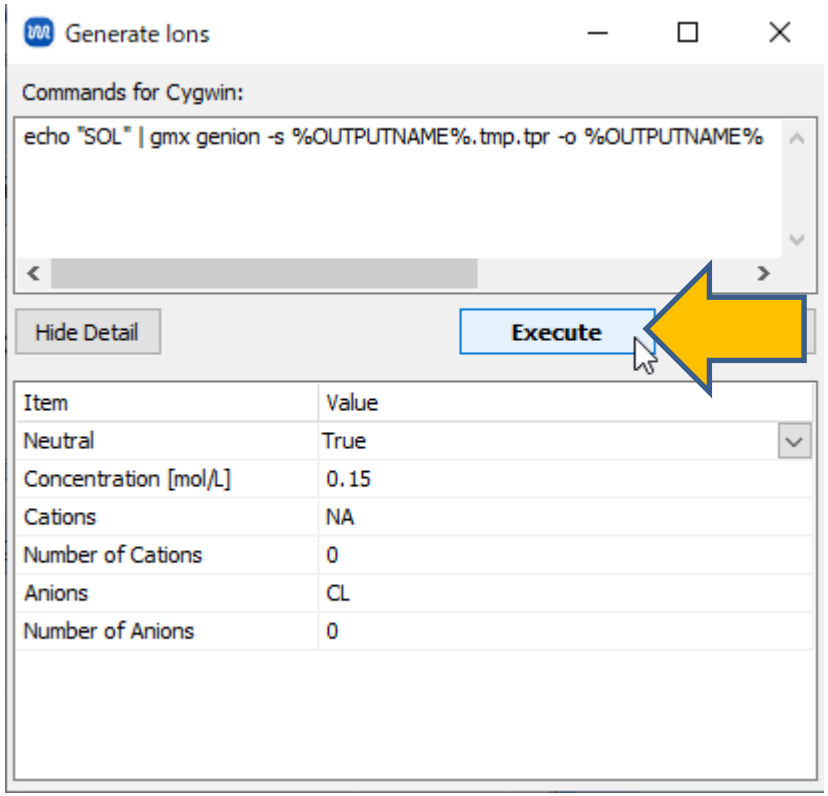


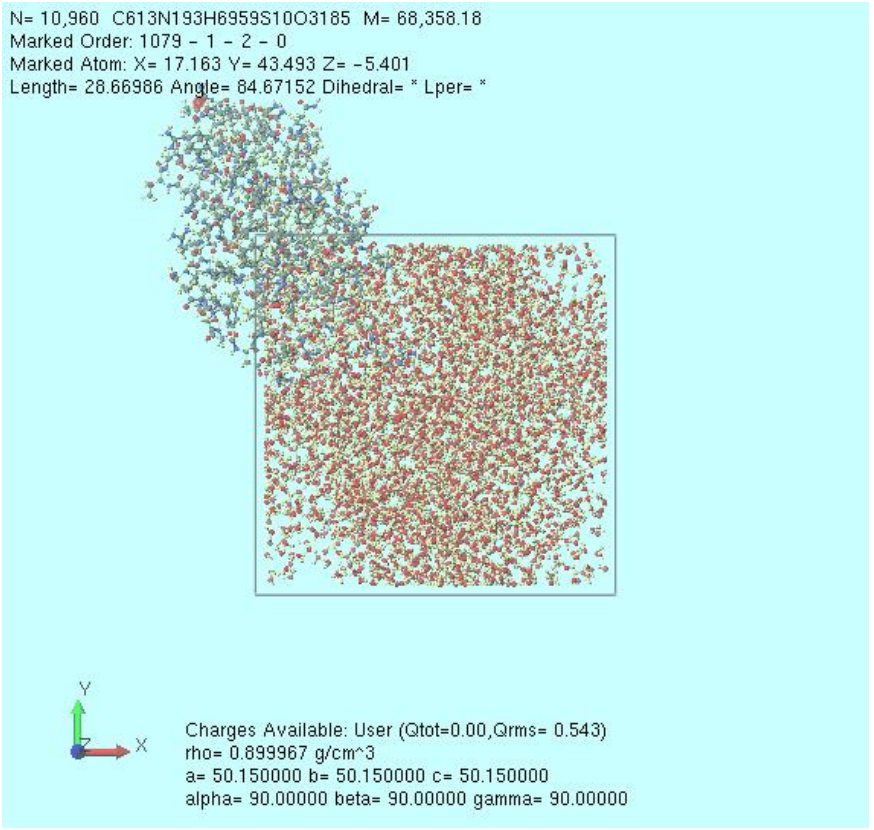


※ The protein coordinates remain fixed to those in the original PDB file, so the structure may cross the cell boundaries. However, this does not lead to any problem as periodic boundary conditions will be applied in the calculation.

A. Modeling of the System

A. Click **MD | Generate Ions** and **Yes** when the warning message appears.
B. Click **Execute**.





B. Execution of Calculation (Energy minimization with protein position restraints)

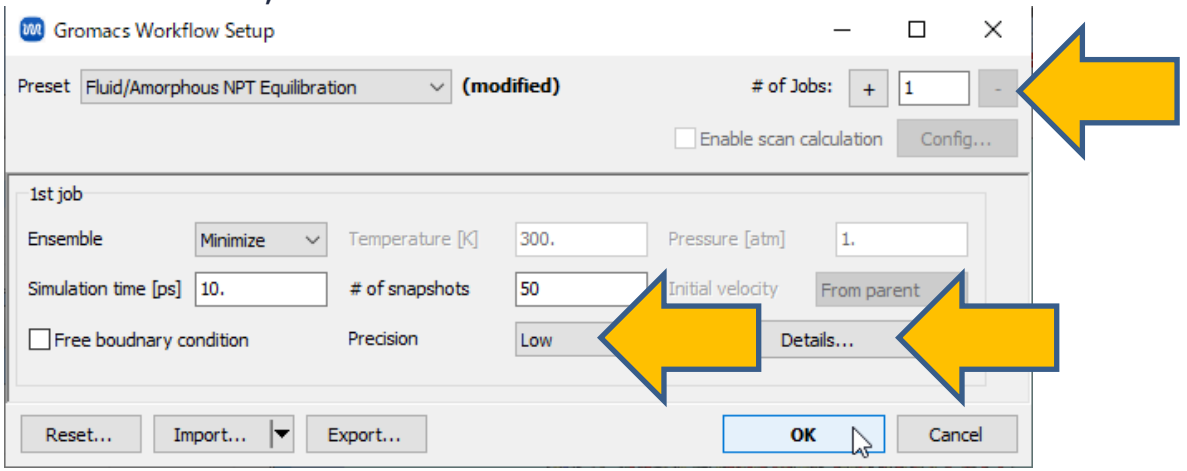
A. Select **Gromacs** from **Solver**, and open **(Workflow Setup).**

B. Click **No** when the message of '…Do you want to assign charges now?' appears.

C. Click **OK** in the window of **Assigned force field parameters**.
Click **OK** as each message appears in order.
'NOTE:…' and 'Assigned force field parameters.' are displayed.

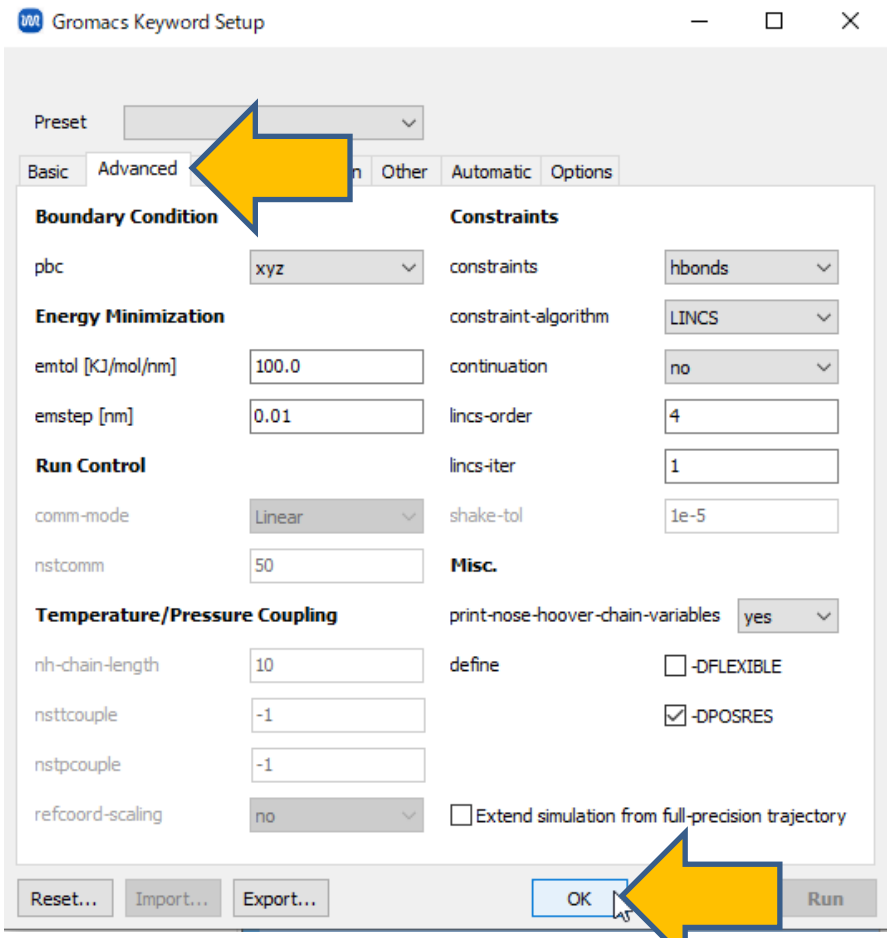
D. In the **Gromacs Workflow Setup** window, click the '–' button for # of Jobs twice.
- This energy minimization step may not converge, but it will not adversely affect the subsequent NVT simulation. Due to current Winmostar specifications, if the minimization fails to converge, the workflow will be interrupted. Therefore, only the energy minimization is executed at this stage. If the workflow is interrupted, the simulation can be resumed later from work1 without any issues.

E. Change **Precision** to **Low**, then click **Details**.



B. Execution of Calculation (Energy minimization with protein position restraints)

A. Switch to the **Advanced** tab, check **-DPOSRES**, and click **OK**.
B. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.



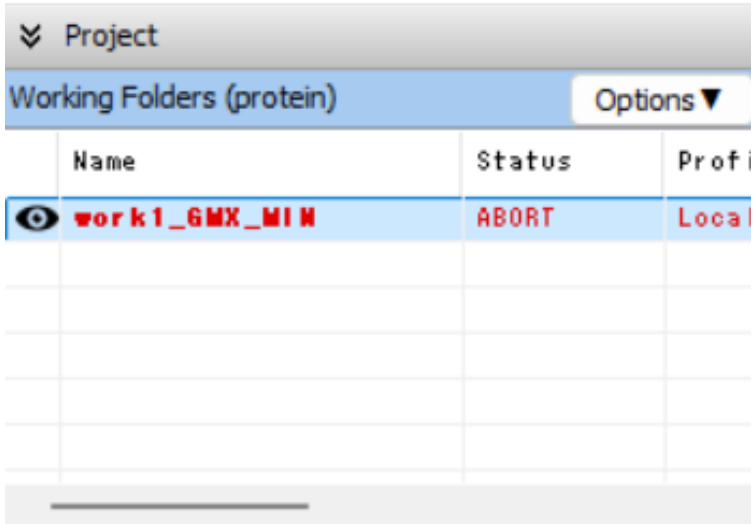
C. Execution of Calculation (Equilibration with protein position restraints)

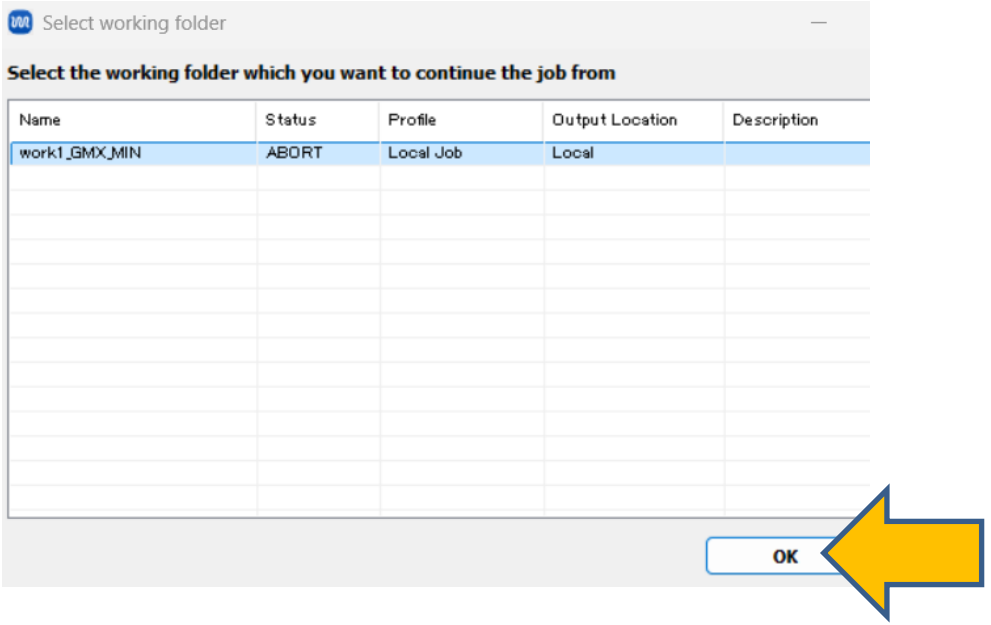
A. After **the status** of **work1_GMX_MIN** in **Working Folders** changes to **ABORT**, open **(Workflow Setup).**

- Even if the job ends with ABORT, continuation is possible if the final structure has been output.

B. If prompted with 'Do you want to continue from previous run?', click **Yes**.

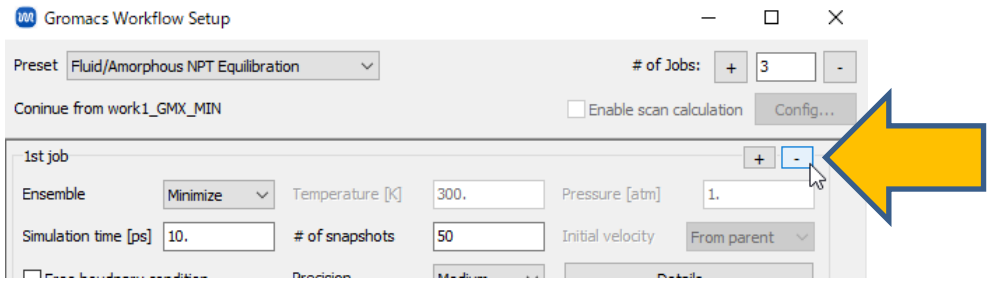
C. Click **OK** in **Select working folder**. Click **Yes** when the message of '…Do you want to ignore and continue?' appears.

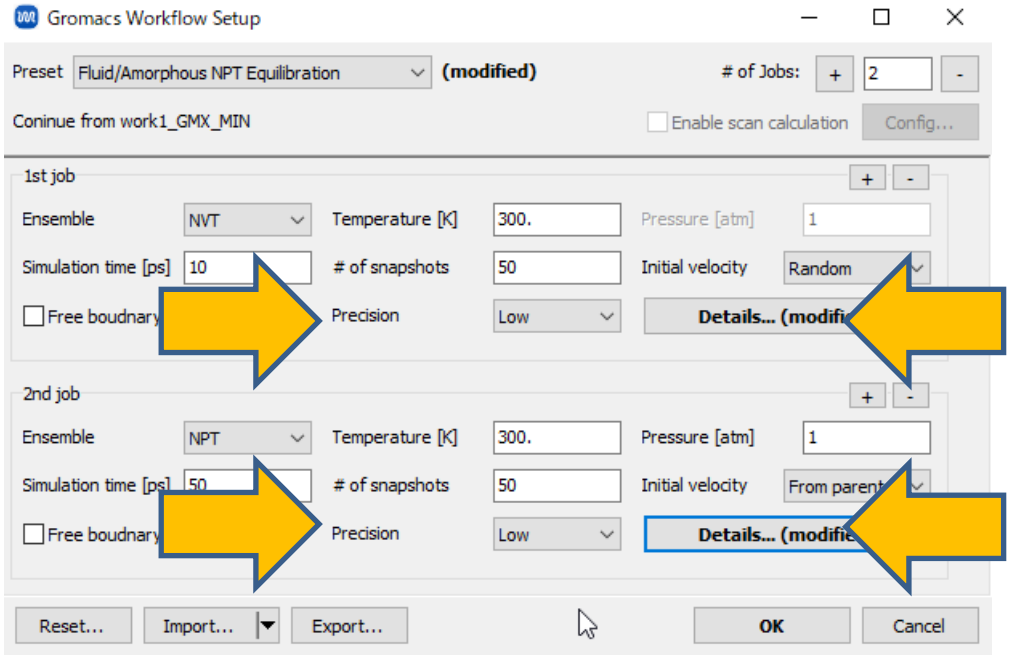




C. Execution of Calculation (Equilibration with protein position restraints)

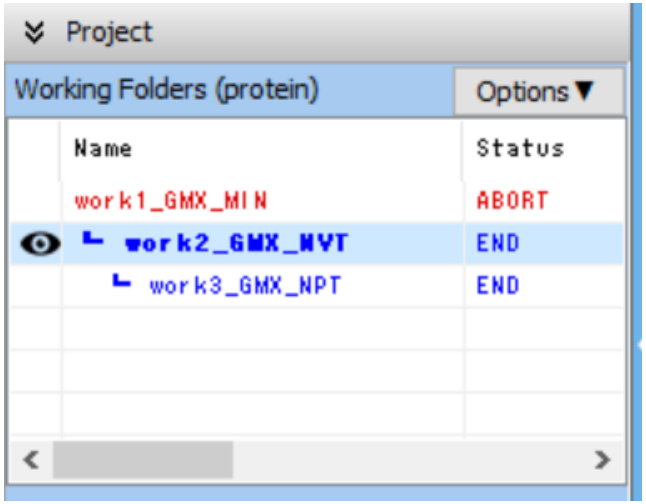
A. Reset the **Preset** to **Fluid/Amorphous NPT Equilibration**.
B. Click the '**-**' button at the top right of the **1st job** row.
C. Set the **Precision** of both the **1st** and **2nd jobs** to **Low**.
D. Click **Details** for the **1st job**, check **-DPOSRES**, and click **OK**.
E. Click **Details** for the **2nd job**, check **-DPOSRES**, and click **OK**.
F. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.

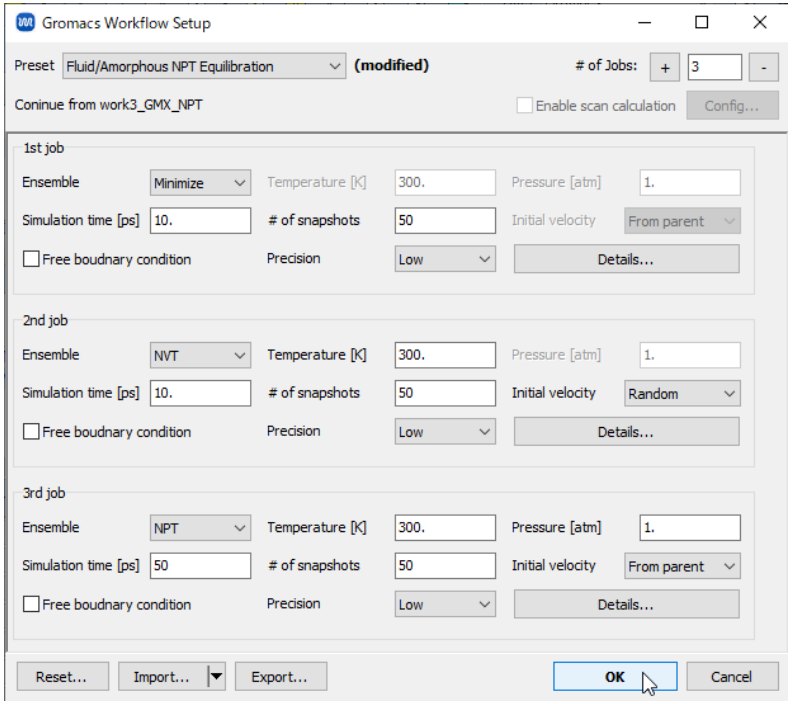




D. Execution of Calculation (Equilibration)

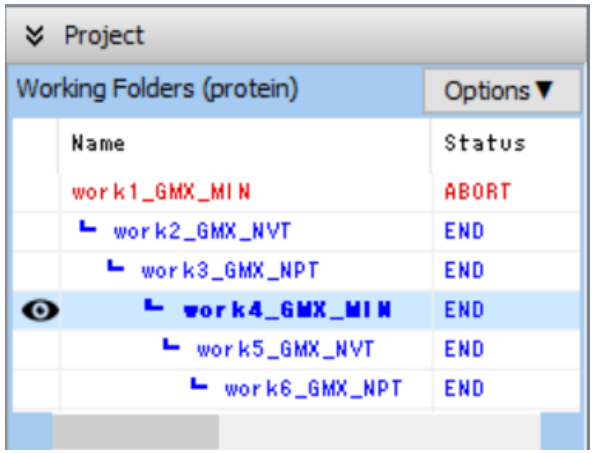
A. Once **the status** of work3_GMX_NPT changes to **END**, click **(Workflow Setup)** again.
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.
C. Select work3_GMX_NPT and click **OK**.
D. Reset the **Preset** to **Fluid/Amorphous NPT Equilibration**.
E. Set the **Precision** of the **1st , 2nd and 3rd jobs** to **Low**.
F. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.

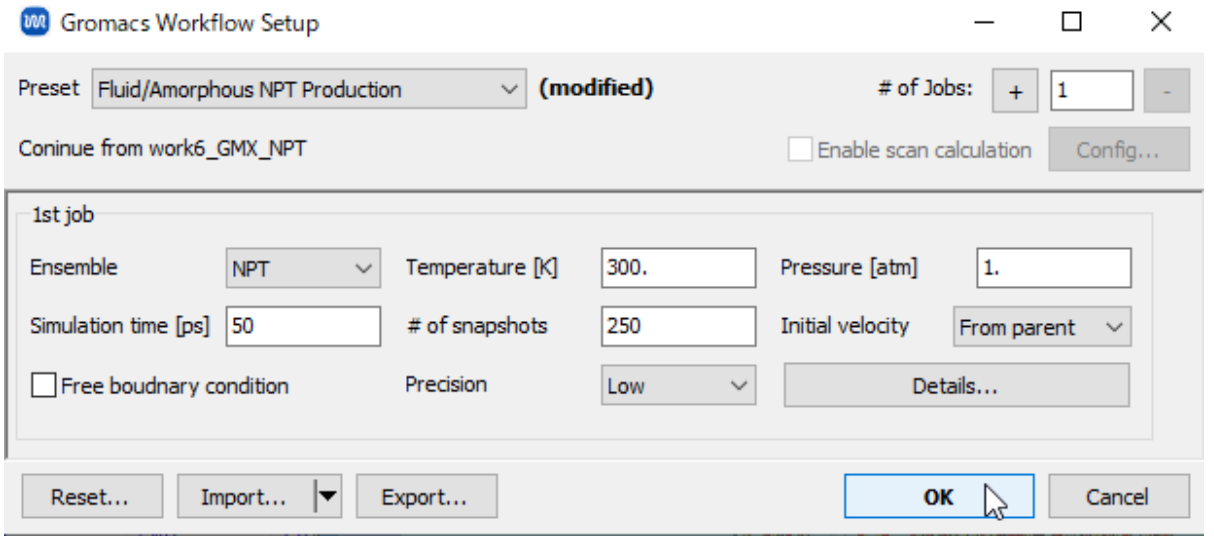




E. Execution of Calculation (Main Calculation)

A. Once **the status** of work6_GMX_NPT changes to **END**, click **(Workflow Setup)** again.
B. If prompted with 'Do you want to continue from previous run?', click **Yes**.
C. Select work6_GMX_NPT and click **OK**.
D. Change **Preset** to **Fluid/Amorphous NPT Production.**
E. Adjust **Precision** and **Simulation time** as needed. In this tutorial, set **Precision** to **Low**.
F. Click **OK**, then make appropriate settings in **Job Setting** window and click **Run**.



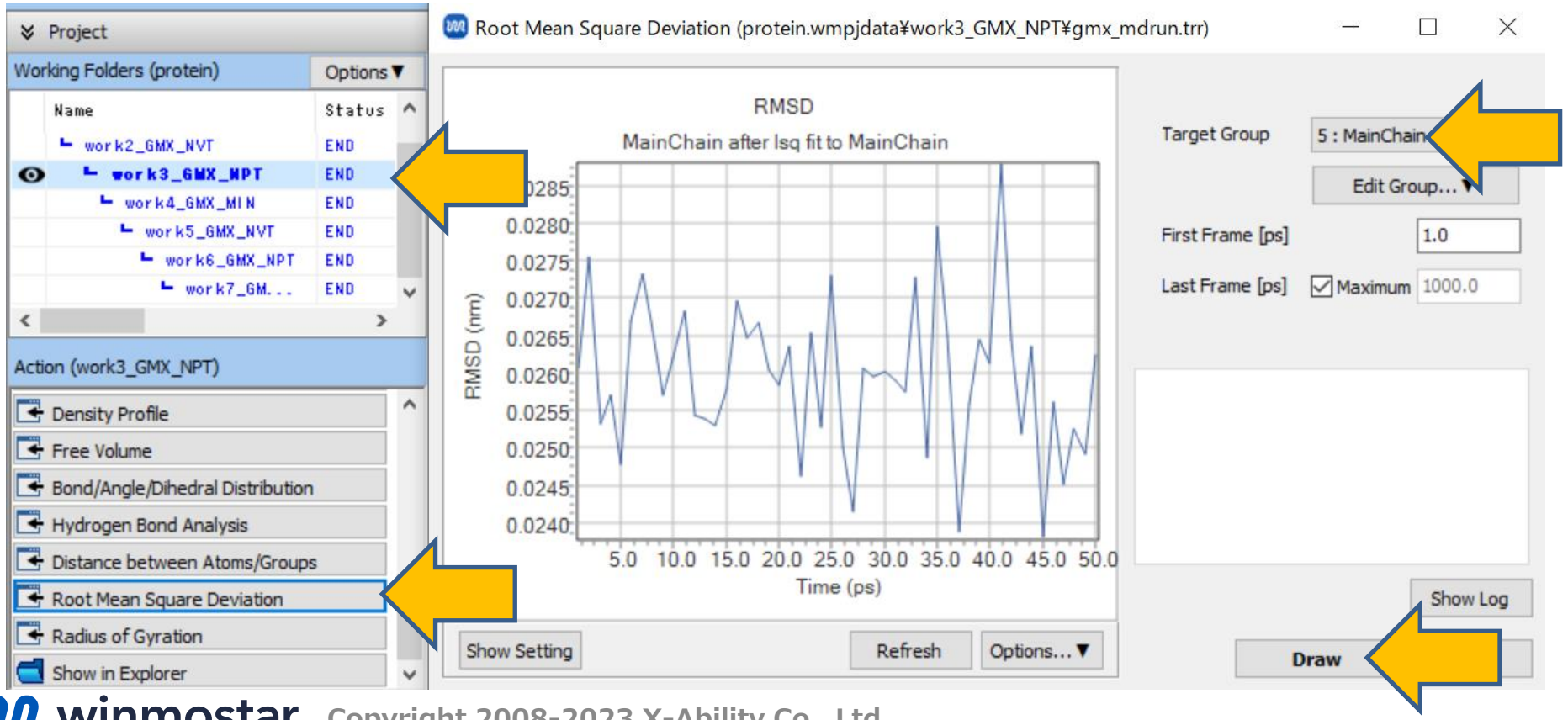


F. Analysis of Results

This section explains how to confirm that the protein is properly restrained.

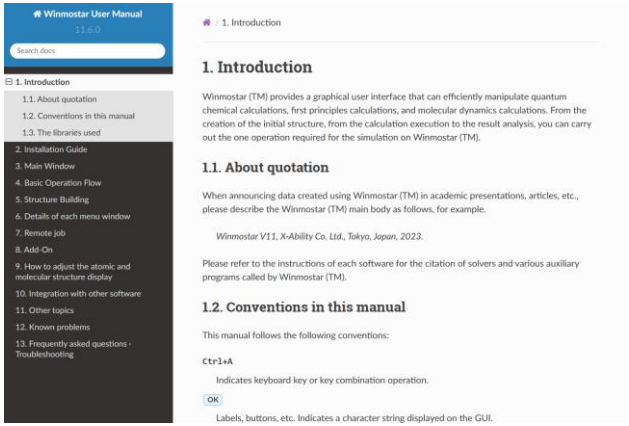
A. In the **Working Folders**, click the job you want to check (e.g., work3_GMX_NPT), then select **Root Mean Square Deviation** from the **Action** menu.

B. Select '5: Main Chain' in the **Target Group** and click **Draw**.



Finally

- For detailed information on each feature, please refer to Winmostar User Manual.



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Scenes from Winmostar Training Session

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