CHARMM-GUI

Effective Simulation Input Generator and More

CHARMM is a versatile program for atomic-level simulation of many-particle systems, particularly macromolecules of biological interest. - M. Karplus

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1.

CHARMM-GUI

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Since its original development in 2006, CHARMM-GUI has proven to be an ideal web-based platform to interactively build complex systems and prepare their inputs with well-established and reproducible simulation protocols for state-of-the-art biomolecular simulations using widely used simulation packages such as CHARMM, NAMD, GROMACS, AMBER, GENESIS, LAMMPS, Desmond, and OpenMM. The CHARMM-GUI development project has been widely adopted for various purposes and now contains a number of different modules designed to set up a broad range of biomolecular simulation systems in Input Generator. Many original modules were developed as an in-house effort, but we have established close collaborations with the developers of CHARMM and other MD simulation packages for addition of newer modules.

Our philosophy in CHARMM-GUI development is less about providing the nuts and bolts of molecular modeling, but instead focused on helping users to achieve a task, such as building a membrane system or solvating a protein, by providing a streamlined interface. This design principle helps us to think of the workflow critically when designing the interface, which leads CHARMM-GUI to be accessible to users with little experience in modeling tools and remains useful to experts, especially for batch generation of systems. CHARMM-GUI has been used by many researchers, and it is a well-recognized tool in the biomolecular modeling and simulation communities (see Google Scholar Citations).

The CHARMM-GUI development project is still ongoing. These functionalities are not only based on requests from general users and developers, but also on an emerging need for a unified platform to prepare and execute various advanced simulation approaches that have been developed and will be developed by many developers in diverse simulation communities and packages. CHARMM-GUI will continue to help expert and non-expert researchers from a broader range of the modeling and simulation community to build the complex biomolecular systems of their interest and prepare the input files for any general and advanced modeling and simulation through the large and unique scope of CHARMM-GUI functionality. It will also provide an effective one-stop online resource for the biomedical research community to carry out innovative and novel biomolecular modeling and simulation research.

Visit our COVID-19 Archive for collection of SARS-CoV-2 protein systems.
Follow CHARMM-GUI on Twitter: https://twitter.com/CharmmGui.

CHARMM-GUI CECAM School in Toulouse, France (September 05-10, 2021)


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2.
Input Generator
User Profile
One easiest way to support CHARMM-GUI is to cite the CHARMM-GUI main paper as well as the papers of the modules used in users' publications. Please see Citations for details.
Since most modules start with PDB Reader, it is strongly recommended to read the PDB Reader page and to see the PDB Reader demo in Video Demo.
Job Retriever
Facilitates recovery of jobs, when the Job ID is known
PDB Reader
Read a PDB file (RCSB or CHARMM formats) into CHARMM
Glycan Reader & Modeler
Read carbohydrate structures from a PDB file into CHARMM and/or model user-specified N-/O-glycan or glycan-only structure(s)
Ligand Reader & Modeler
Generate various ligand structures using the CHARMM force field
Glycolipid Modeler
Provide various glycolipid structure and PSF files
LPS Modeler
Provide various lipopolysaccharide (LPS) structure and PSF files
Nanomaterial Modeler
Generate various nanomaterial systems for molecular dynamics simulation
Multicomponent Assembler
Combine PSF/CRD of non-membrane molecules into a heterogeneous system
Solvator
Solvate globular protein, or generate various shapes of water box
Solution Builder (new Quick MD Simulator)
Setup subsequent steps for molecular dynamics simulations of globular proteins
Drude Prepper
Prepare the systems ready for simulations with the Drude polarizable force fields from an identical system equilibrated with the CHARMM36 non-polarizable additive force fields

- Free Energy Calculator
- LBS Finder & Refiner
- Ligand Designer
- MAP Utilizer
- DEER Facilitator
- NMR Structure Calculator
- PBEQ Solver
- Implicit Solvent Modeler
- Boundary Potential Utilizer
- GCMC/BD Ion Simulator

Coulombic and van der Waals interactions. By simply changing a variable of *nmc* in the input (*step2.2_ions.inp*), you can perform longer MC simulations on your local machine.

Please note that

- If you are not familiar with the first PDB reading step, please first watch these video demos.

Reference for Solution Builder:
S. Jo, T. Kim, V.G. Iyer, and W. Im (2008)
CHARMM-GUI: A Web-based Graphical User Interface for CHARMM. *J. Comput. Chem. 29:1859-1865*
J. Lee, X. Cheng, J.M. Swails, M.S. Yeom, P.K. Eastman, J.A. Lemkul, S. Wei, J. Buckner, J.C. Jeong, Y. Qi, S. Jo, V.S. Pande, D.A. Case, C.L. Brooks III, A.D. MacKerell Jr, J.B. Klauda, and W. Im (2016)
CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. *J. Chem. Theory Comput. 12:405-413*
J. Lee, M. Hitzenberger, M. Rieger, N.R. Kern, M. Zacharias, and W. Im (2020)
CHARMM-GUI supports the Amber force fields. *J. Chem. Phys. 153:035103*

Protein Solution System 3. enter “2QMT”

Download PDB File: 2QMT Download Source: RCSB

Upload PDB File: 選択... ファイルが選択されていません。

PDB Format: PDB PDBx/mmCIF CHARMM

Water Box Only System

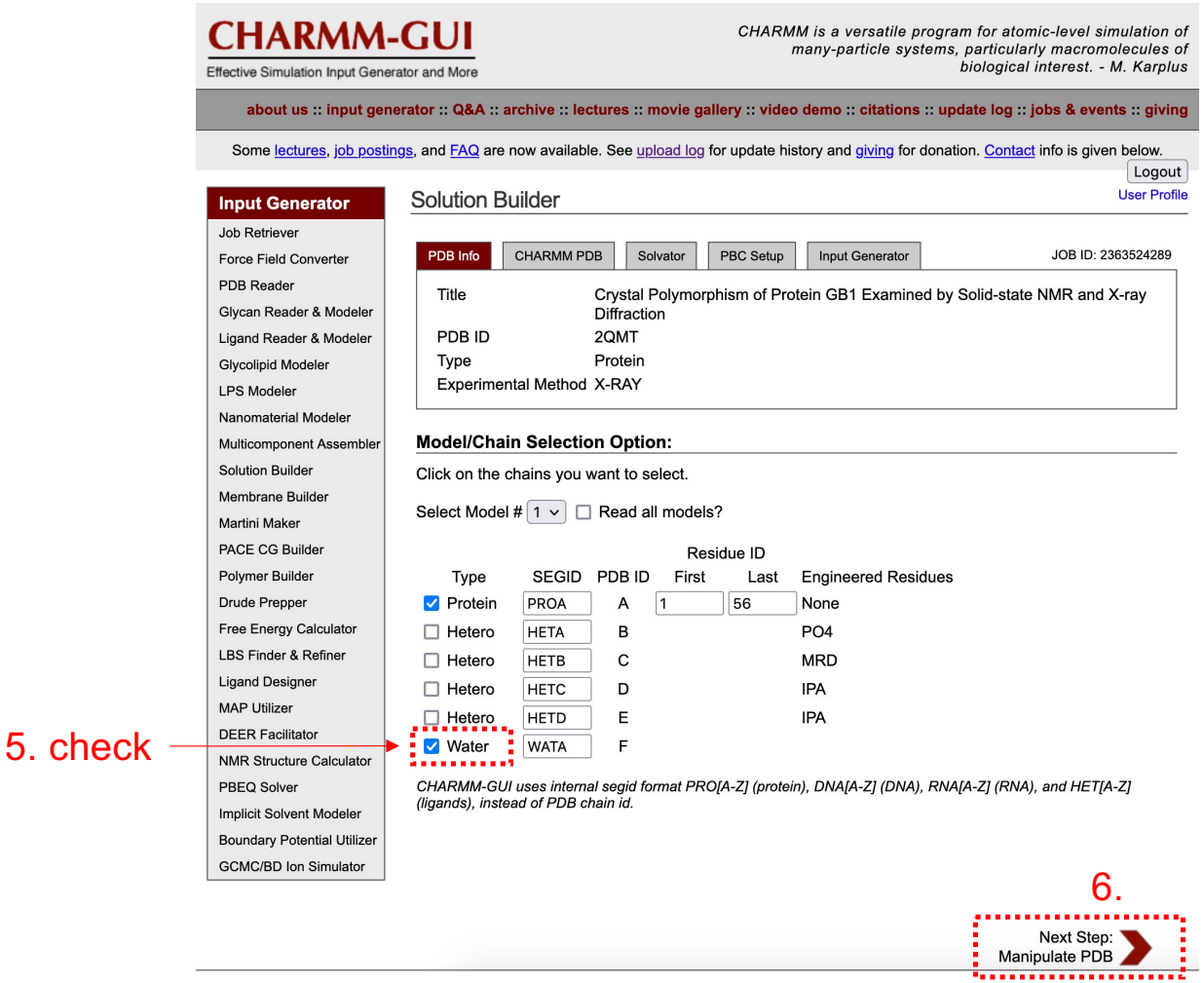
Select Water Box Type: Rectangular

X: Å Y: Å Z: Å

Include Ions

4.

Next Step:
Select Model/Chain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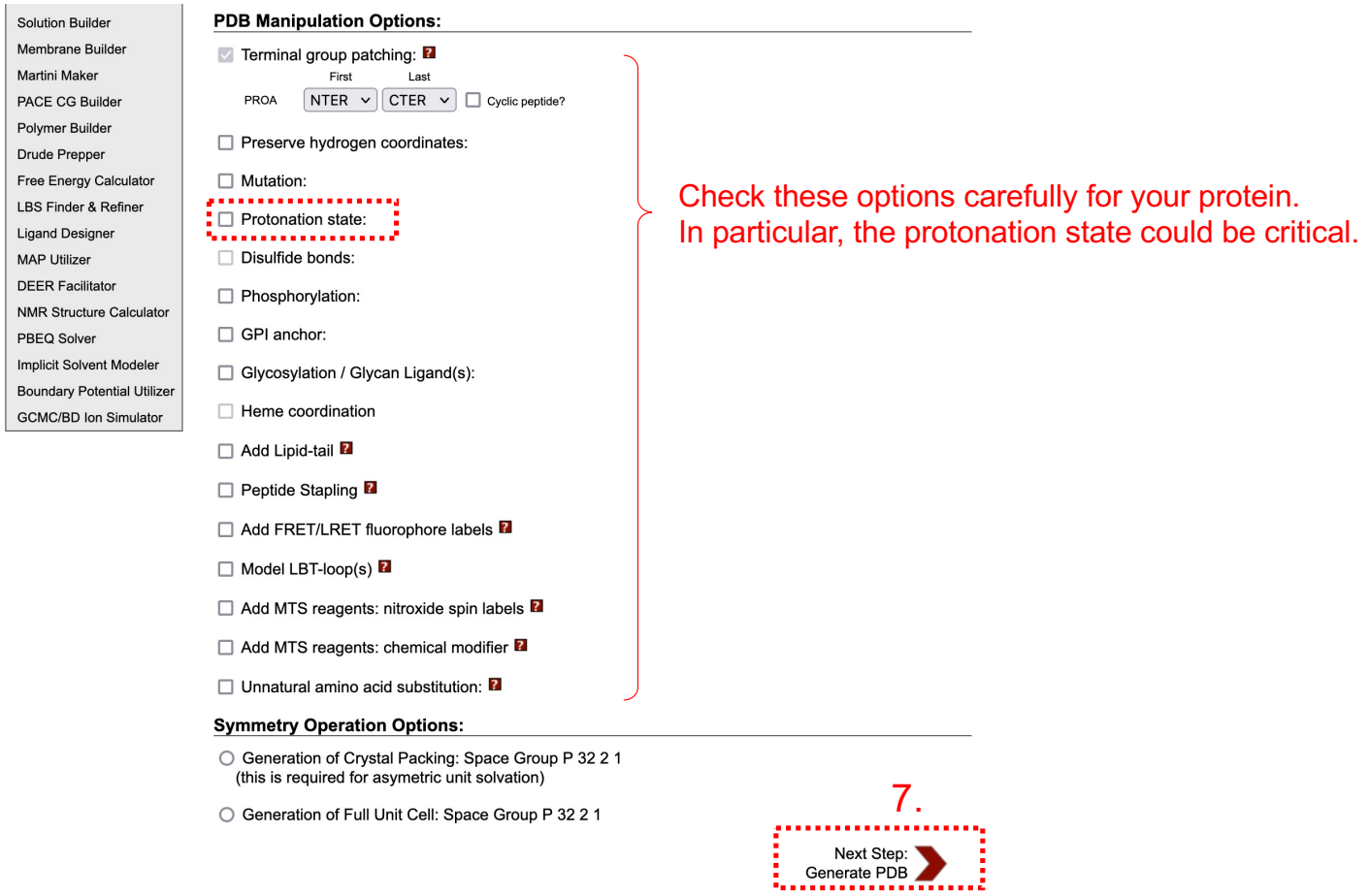
Ligand Designer
MAP Utilizer
DEER Facilitator
NMR Structure Calculator
PBEQ Solver
Implicit Solvent Modeler
Boundary Potential Utilizer
GCMC/BD Ion Simulator
Solution Builder
PDB Info
CHARMM PDB
Solvator
PBC Setup
Input Generator
JOB ID: 2363524289
Title
Crystal Polymorphism of Protein GB1 Examined by Solid-state NMR and X-ray Diffraction
PDB ID
2QMT
Type
Protein
Experimental Method
X-RAY
Model/Chain Selection Option:
Click on the chains you want to select.
Select Model # 1
Read all models?
Residue ID
Type
SEGID
PDB ID
First
Last
Engineered Residues
Protein
PROA
A
1
56
None
Hetero
HETA
B
PO4
Hetero
HETB
C
MRD
Hetero
HETC
D
IPA
Hetero
HETD
E
IPA
Water
WATA
F
CHARMM-GUI uses internal segid format PRO[A-Z] (protein), DNA[A-Z] (DNA), RNA[A-Z] (RNA), and HET[A-Z] (ligands), instead of PDB chain id.
Next Step: Manipulate PDB

5. check

6.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Ligand Designer
MAP Utilizer
DEER Facilitator
NMR Structure Calculator
PBEQ Solver
Implicit Solvent Modeler
Boundary Potential Utilizer
GCMC/BD Ion Simulator
PDB Manipulation Options:
Terminal group patching:
First
Last
PROA
NTER
CTER
Cyclic peptide?
Preserve hydrogen coordinates:
Mutation:
Protonation state:
Disulfide bonds:
Phosphorylation:
GPI anchor:
Glycosylation / Glycan Ligand(s):
Heme coordination
Add Lipid-tail
Peptide Stapling
Add FRET/LRET fluorophore labels
Model LBT-loop(s)
Add MTS reagents: nitroxide spin labels
Add MTS reagents: chemical modifier
Unnatural amino acid substitution:
Check these options carefully for your protein.
In particular, the protonation state could be critical.
Symmetry Operation Options:
Generation of Crystal Packing: Space Group P 32 2 1
(this is required for asymetric unit solvation)
Generation of Full Unit Cell: Space Group P 32 2 1
7.
Next Step:
Generate PDB

- PDB Reader
- Glycan Reader & Modeler
- Ligand Reader & Modeler
- Glycolipid Modeler
- LPS Modeler
- Nanomaterial Modeler
- Multicomponent Assembler
- Solution Builder
- Membrane Builder
- Martini Maker
- PACE CG Builder
- Polymer Builder
- Drude Prepper
- Free Energy Calculator
- LBS Finder & Refiner
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- MAP Utilizer
- DEER Facilitator
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- Boundary Potential Utilizer
- GCMC/BD Ion Simulator

PDB Info | CHARMM PDB | Solvator | PBC Setup | Input Generator

JOB ID: 2363672375

download.tgz

Original PDB File: 2QMT.cif (view structure)
Individual Chains: 2qmt_proa.pdb
2qmt_wata.pdb
CHARMM Input: step1_pdbreader.inp
CHARMM Output: step1_pdbreader.out
CHARMM PDB: step1_pdbreader.pdb (view structure)
CHARMM CRD: step1_pdbreader.crd
CHARMM PSF: step1_pdbreader.psf

Computed Energy:

Please beware of that the computed energy is CHARMM single-point energy and is displayed to make sure all the coordinates are defined.

```
ENER ENR:  Eval#     ENERgy      Delta-E         GRMS
ENER INTERN:          BONDs       ANGLes       UREY-b    DIHEdrals    IMPRopers
ENER CROSS:           CMAPs        PMF1D        PMF2D       PRIMO
ENER EXTERN:        VDWaals         ELEC       HBONds          ASP         USER
 ---------       ---------    ---------    ---------    ---------    ---------
ENER>       0   -351.24746      0.00000     22.31013
ENER INTERN>      93.88156    133.40069     22.73769    530.20829      3.60776
ENER CROSS>      -33.38607      0.00000      0.00000      0.00000
ENER EXTERN>     730.56192  -1832.25931      0.00000      0.00000      0.00000
 ---------       ---------    ---------    ---------    ---------    ---------
```

Waterbox Size Options:

- ○ Specify Waterbox Size
- ◉ Fit Waterbox Size to Protein Size

Waterbox type: Rectangular (Currently, the octahedral box is supported only for CHARMM and NAMD)
Enter Edge Distance: 10.0

padding distance

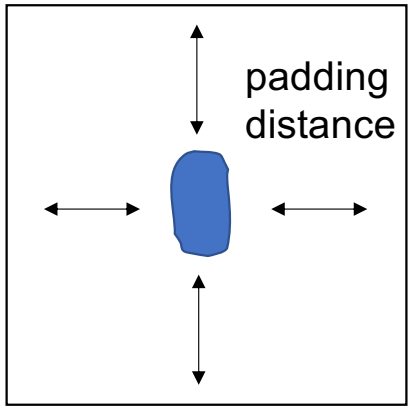
Add Ions:

☑ Include Ions
◉ 0.15 M KCl (ion concentration) Calculate number of ions
○ Add neutralizing ions
22 positive ions and 18 negative ions will be generated. Note that this is the estimated ion numbers, so the actual ion numbers may differ.

☑ Ion Placing Method: Monte-Carlo
If your system does not contain nucleic acids, you can use “Distance” for faster ion placement.

8.

Next Step: Solvate Molecule



- DEER Facilitator
- NMR Structure Calculator
- PBEQ Solver
- Implicit Solvent Modeler
- Boundary Potential Utilizer
- GCMC/BD Ion Simulator

System Size:

check the size

Box Type	Rectangle		
Crystal Type	CUBIC		
System Size	A	60	Dimension along the A (X) axis
	B	60	Dimension along the B (Y) axis
	C	60	Dimension along the C (Z) axis
Crystal Angle	Alpha	90.0	Angle between the axis B and C
	Beta	90.0	Angle between the axis A and C
	Gamma	90.0	Angle between the axis A and B
# of Ions	POT	22	
	CLA	18	

Periodic Boundary Condition Options:

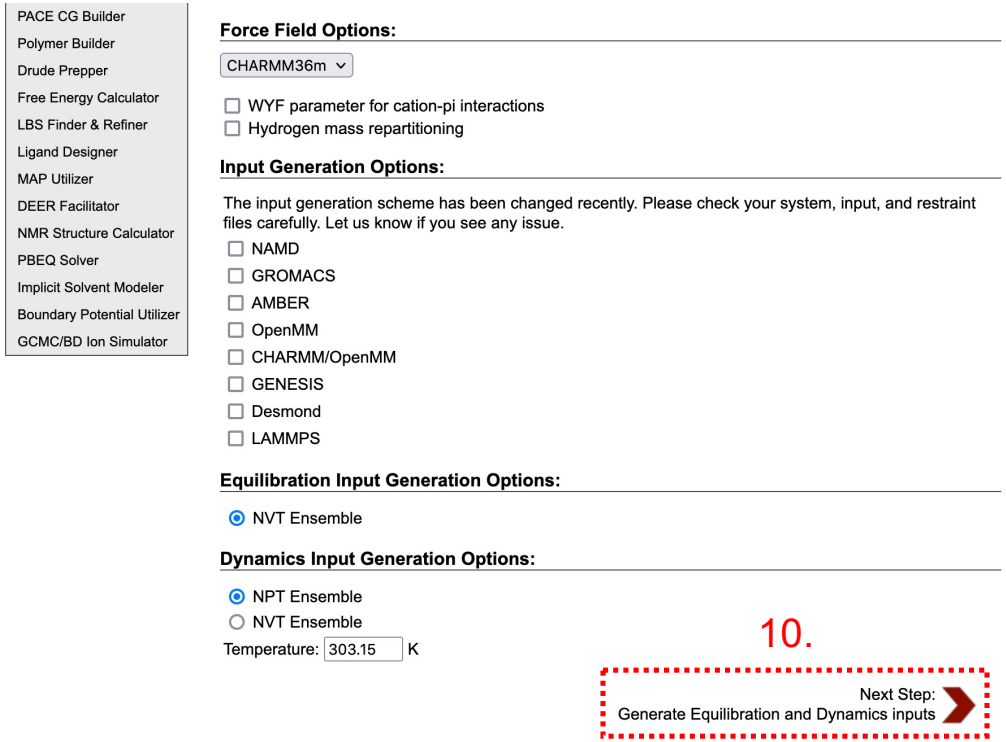
- (•) Generate grid information for PME FFT automatically
- ( ) Explicit grid information for PME FFT

X Y Z

[ ] [ ] [ ]

9.

Next Step:
Setup Periodic Boundary Condition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Ligand Designer
MAP Utilizer
DEER Facilitator
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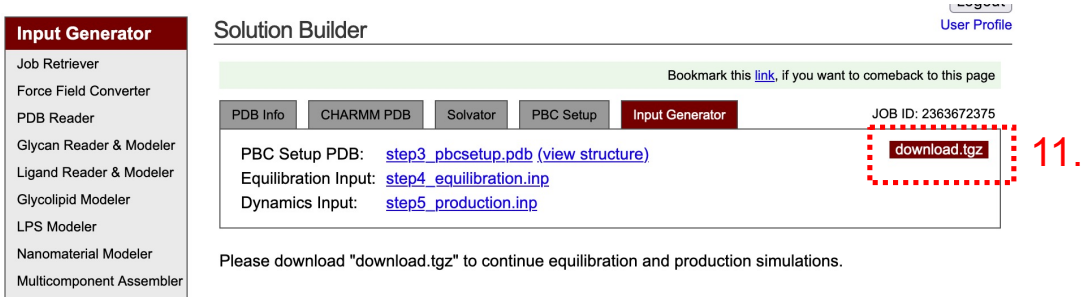
PBEQ Solver
Implicit Solvent Modeler
Boundary Potential Utilizer
GCMC/BD Ion Simulator
Force Field Options:
CHARMM36m
WYF parameter for cation-pi interactions
Hydrogen mass repartitioning
Input Generation Options:
The input generation scheme has been changed recently. Please check your system, input, and restraint files carefully. Let us know if you see any issue.
NAMD
GROMACS
AMBER
OpenMM
CHARMM/OpenMM
GENESIS
Desmond
LAMMPS
Equilibration Input Generation Options:
NVT Ensemble
Dynamics Input Generation Options:
NPT Ensemble
NVT Ensemble
Temperature: 303.15 K
10.
Next Step:
Generate Equilibration and Dynamics inputs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Solution Builder
User Profile
Bookmark this link, if you want to comeback to this page
PDB Info
CHARMM PDB
Solvator
PBC Setup
Input Generator
JOB ID: 2363672375
PBC Setup PDB: step3_pbcsetup.pdb (view structure)
Equilibration Input: step4_equilibration.inp
Dynamics Input: step5_production.inp
download.tgz
Please download "download.tgz" to continue equilibration and production simulations.

11.