Protein Data Bank
web site

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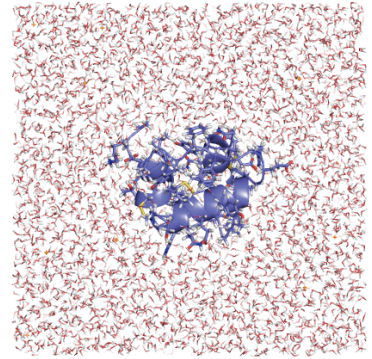
PDB file

VMD/PSFGEN
CHARMM
CHARMM-GUI

Add hydrogen
Add water
Add ions



Target system

CHARMM developers
website

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Topology file ①

Parameter file ②

PSF file ③

PDB file ④

GENESIS
Generalized-ensemble simulation system

Input section

① ② ③ ④

```
[INPUT]
topfile  = top_all36_prot.rtf, top_all36_lipid.rtf  # topology file
parfile  = par_all36_prot.prm, par_all36_lipid.prm  # parameter file
strfile  = toppar_water_ions.str  # stream file
psffile  = ionized.psf            # protein structure file
pdbfile  = ionized.pdb            # initial structure
reffile  = ionized.pdb            # reference coordinates for restraints

[OUTPUT]
dcdfile  = min.dcd          # DCD trajectory file
rstfile  = min.rst          # restart file

[ENERGY]
forcefield       = CHARMM   # CHARMM force field
electrostatic    = PME      # Particle Mesh Ewald method
switchdist       = 10.0     # switch distance
cutoffdist       = 12.0     # cutoff distance
pairlistdist     = 13.5     # pair-list distance
```

Control file of GENESIS