All Atom Setup

- Load your protein (+ coordinated ions..) PDB of choice into VMD
- Extensions → Modeling → **Automatic PSF Builder**
    - Click "Load Input Files". (Default input files are almost always OK)
    - Select 'Everything,' and click "Guess and split chains using current selection"
    - Look at the segments it created for you. Make any changes
        - I usually rename them to simplify things down the line (i.e., "AP1" > "A")
        - Also make sure there's no overlap in chain name. (If there is, fix that in your starting PDB with Phenix and start over)
    - Click "create chains," and accept the popups.
    - Check that the patches make sense, if any.
    - Click "Apply patches and finish PSF/PDB"
    - **OUTPUT:** yourfile_autopsf.pdb, yourfile_autopsf.psf
- Extensions → Modeling → **Add Solvation Box**
    - Uncheck "waterbox only," if needed, and make sure your outputs (above) are loaded
    - Change "output" to yourfile_S
    - Check "rotate to minimize volume," and "Use Molecule Dimensions"
    - Add a reasonable padding to your molecule. For me, 12.5A in all boxes
    - Click Solvate. **OUTPUT:** yourfile_S.pdb, yourfile_S.psf
- Extensions → Modeling → **Add Ions**
    - Make sure your outputs are loaded. Change "output" to "yourfile_SI"
    - Select salt of choice (for me, KCl for cytosolic).
    - Select "Neutralize and set xxx concentration to …" and your conc of choice (for me, 0.1M).
    - Click "Autoionize." **OUTPUT:** yourfile_SI.pdb, yourfile_SI.psf
- Center your molecule in 3D space and measure your box boundaries
    - Extensions → **Tk Console.** Make sure yourfile_SI.psf is the "T" top molecule selected
    - Type "set sel [atomselect top all]", enter
    - Type "set coords [measure center $sel]", enter
    - Type "$sel moveby [vecinvert $coords]", enter
    - Type "$sel writepdb yourfile_SIC.pdb", enter
    - Type "measure minmax $sel"
        - Add the absolute value of each coordinate together. Round to the nearest number
    - In terminal, open yourfile-min.conf in a text editor, i.e. "vim yourfile-min.conf"
        - Use rounded numbers for the cellBasisVector X, Y, Z measurements of the periodic boundary conditions. cellOrigin remains 0.00, 0.00, 0.00. Save and exit editor.
- Back in VMD, Restrain your protein backbone from moving during minimization
    - Load your centered pdb file, yourfile_SIC.pdb, from above
        - File → New molecule, browse → yourfile_SIC.pdb → Load
    - Extensions → **Tk Console**
    - Type "set sel [atomselect top "protein and backbone"]", enter
    - Type "$sel set beta 10"
    - Type "set sel [atomselect top all]"
    - Type "$sel writepdb yourfile_SICR.pdb"

Close VMD

Minimization

- Collect necessary files
  - **Input files:** yourfile_SICR.pdb, yourfile_SI.psf
  - **Minimization config file**, named yourfile-min.conf
  - **Parameters**: par_all35m_prot.prm, toppar_water_ions.str
  - **Submit files**: min-job-submit.sbatch
- Edit config file
  - Change blurb at top to describe your experiment, including date and molecule and goal
  - Change Input files to match yours:
    - coordinates yourfile_SICR.pdb
    - structure yourfile_SI.psf
  - Change Output Controls / outputname to yourfile-min
  - Change restraint setup / Consref and restraint setup/ConsKFile to yourfile_SICR.pdb
  - Set periodic boundary conditions appropriately
    - ***UPDATE THIS GUIDANCE!***
    - Take minmax of the SIC pdb. Add absolute value of each coord X, Y, Z and round up to the nearest whole number.
    - Set cell origin = 0
- Edit submit script and submit job
  - Edit job name, output, and NAMD file input and file output names to yourfile-min
  - Submit! sbatch min-job-submit.sbatch
    - Should take < 10min
    - Check after about 30 seconds to make sure it's running OK.

Heat/Equilibration

- Collect necessary files
  - **Input files:** yourfile_SICR.pdb, yourfile_SI.psf
  - **Minimization config file**, named yourfile-hEQ.conf
  - **Parameters**: par_all35m_prot.prm, toppar_water_ions.str
  - **Submit files**: hEQ-job-submit.sbatch
- Get coordinates from last frame of minimization
  - Open yourfile_SI.psf, and open yourfile-min.dcd into the psf
    - Make sure yourfile_SI.psf is selected in the "load files for" dropdown before browsing for the yourfile-min.dcd file