Supplementary Figure 1. Script to align simulation snapshots with the template (starting structure) in YASARA. Each aligned snapshot is subsequently saved as a new PDB.

```
clear


#"i" controls the number of snapshots, in this case 11 snapshots were
#generated (one every 2 ns and including the template at time zero).
i=0
while i < 22000
  Loadsce (Macrotarget)
  sim = FileSize (MacroTarget)(i).sim
  TempCtrl Rescale
  #In this case AMBER99 was used as force field
  Forcefield Amber99
  #Change the cut-off to standard settings according to your software
  #version
  Cutoff 7.86
  Longrange Coulomb
  Boundary Periodic

  console On
  if not sim
    ShowMessage 'Could not load snapshot (i)'
  # If there is a snapshot, load it
  LoadSim (MacroTarget)(i)
  Sim Off
  simtime = Time
  ShowMessage 'Analyzing snapshot (0+i) at (0+simtime) ps'
  #In this macro, the .sim files from YASARA are first converted to
  #PDB-files. To do that, we need one object. Check which object
  #numbers are relevant for you. In this case I have object 1,3 and 4.
  JoinObj 3-4,1,Center=Yes
  #Save the joined object as a PDB
  SavePDB 1, (MacroTarget)(i).pdb, format=PDB, Transform=YES
  clear

  console Off


  #Increase i, in this case one snapshot was saved every 2 ns.
  i = i+2000
```

#Now we can start aligning! Set i to the first snapshot (time zero is the template).
i=2000

#Make a table to plot the RMSD for snapshots compared to the template
MakeTab rmsd_tab, Columns = 2

while i < 22000

 #Load the starting structure ("(MacroTarget)0000.pdb") and one snapshot for alignment
 LoadPDB (MacroTarget)0000.pdb, Center = No
 LoadPDB (MacroTarget)(i).pdb, Center = No

 #Align with MUSTANG so that the actual snapshot will share the same coordinates as
 #the template.
 #In this case "molecule A" corresponds to the protein, you might have to adjust this to your
 #case.
 rmsdal,residues,calist() = AlignMol A Obj 2,A Obj 1,Method=MUSTANGPP
 # Calculate RMSD
 rmsd = RMSDMol A Obj 2, A Obj 1
 Tabulate (i)
 Tabulate (rmsd)
 console on
 ShowMessage 'RMSD: (rmsd)'
 #Now delete the template (starting structure)
 DelObj 1
 #Save the aligned snapshot as a new PDB
 SavePDB 2, (MacroTarget)align_(i).pdb, format=PDB, Transform=YES
 DelObj 2

 console off
 #Increase loop variable to repeat for each snapshot
 i = i+2000