Supplemental file

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Figure S1 Consurf analysis of the SNAIL related proteins (SNAIL like, Slug and Scratch protein). A) Sequence alignments of the proteins used showing the conserved (red) to more variant (cyan) amino acids identified. The yellow represents amino acids that had no observable conservation. B) Model of the SNAIL protein showing the amino acids by the color of A (left) with a 180 degree rotation of the Y-axis (right). C) Transparent molecular surfaces of SNAIL using the same color as in A and B but with the addition of DNA (black) showing most of the conserved amino acids found in the DNA binding.
**Figure S2 Z±2 Scanning array information.** A) The averaged potential energy for SNAIL alone from the energy minimized structure for each background at various locations of the two strands (C1-C15 and D21-D35). Potential energy was calculated as the sum of all components (bond, angle, dihedral, planarity, Van der Waals, and Coulombs) using the AMBER03 force field. Error bars represent the standard error of the four background calculations. Results show minimal energetic variations between each structure, suggesting a lack of major structural alterations to SNAIL protein. B-C) Z±2 scores for the DNA consensus sequence at the multiple sites.
Figure S3 DNA_{relz} values at each site on the DNA.
**Figure S4 Role of amino acids Ser 246 and Arg 247 in binding.**

A) The average atom positioning throughout the 500 picosecond simulation for each of the DNA backgrounds overlayed onto of each other for the C4 location of the E-box sequence. Shows the proper distance maintained for hydrogen bonding between Arg 247 and the GG (red) of the CAGGTG E-box sequence, while Ser 246 hydrogen bonds with the backbone for all averages. B) Gel shift assays confirming the importance of amino acids 246 and 247 in binding the E-box sequence. C). Difference between control and multiple consensus location $X_{RZ}$ scores for amino acid Ser 246 (blue) and Arg 247 (red).
Figure S5 Difference between control and multiple consensus location $X_{RZ}$ scores for those amino acids in the DNA recognition locations of the multiple fingers at the multiple locations of the DNA consensus sequence.
Figure S5 (Cont.) Difference between control and multiple consensus location $X_{RZ}$ scores for those amino acids in the DNA recognition locations of the multiple fingers at the multiple locations of the DNA consensus sequence.
Figure S6 Difference between control and multiple amino acid X_{RZ} scores' for the C12-C14 consensus locations.
Figure S7 Heavy atom RMSD difference between control and consensus locations C12-C14.
Figure S8 Representative plot of energy (A) and carbon alpha RMSD (B) over the course of molecular dynamics simulations on the four DNA base pair backgrounds.
**6bp Scanning Array Macro**

# Setup of DNA scanning array for six base pair consensus, creating 30 scenes for each DNA set, yielding 120 scenes for simulation.

# This is the only place the consensus needs changed

First = 'DC'
Second = 'DA'
Third = 'DG'
Fourth = 'DG'
Fifth = 'DT'
Six = 'DG'

Cfirst = 'DG'
Csecond = 'DT'
CThird = 'DC'
CFourth = 'DC'
CFifth = 'DA'
CSix = 'DC'

# No changes needed after this point for array generation

# Simulation cell and conditions
SimSpeed Normal
ForceField AMBER03,SetPar=No
Interactions Bond,Angle,Dihedral,Planarity,Coulomb,VdW
CleanAll
Boundary periodic

# Setting up the first scene

#A
LoadSce (macrotarget).sce
SwapRes 1, DA, Isomer=L
SwapRes 2, DA, Isomer=L
SwapRes 3, DA, Isomer=L
SwapRes 4, DA, Isomer=L
SwapRes 5, DA, Isomer=L
SwapRes 6, DA, Isomer=L
SwapRes 7, DA, Isomer=L
SwapRes 8, DA, Isomer=L
SwapRes 9, DA, Isomer=L
SwapRes 10, DA, Isomer=L
SwapRes 11, DA, Isomer=L
SwapRes 12, DA, Isomer=L
SwapRes 13, DA, Isomer=L
SwapRes 14, DA, Isomer=L
SwapRes 15, DA, Isomer=L
SwapRes 16, DA, Isomer=L
SwapRes 17, DA, Isomer=L
SwapRes 18, DA, Isomer=L
SwapRes 19, DA, Isomer=L
SwapRes 20, DA, Isomer=L
SwapRes 21, Dt, Isomer=L
SwapRes 22, Dt, Isomer=L
SwapRes 23, Dt, Isomer=L
SwapRes 24, Dt, Isomer=L
SwapRes 25, Dt, Isomer=L
SwapRes 26, Dt, Isomer=L
SwapRes 27, Dt, Isomer=L
SwapRes 28, Dt, Isomer=L
SwapRes 29, Dt, Isomer=L
SwapRes 30, Dt, Isomer=L
SwapRes 31, Dt, Isomer=L
SwapRes 32, Dt, Isomer=L
SwapRes 33, Dt, Isomer=L
SwapRes 34, Dt, Isomer=L
SwapRes 35, Dt, Isomer=L
SwapRes 36, Dt, Isomer=L
SwapRes 37, Dt, Isomer=L
SwapRes 38, Dt, Isomer=L
SwapRes 39, Dt, Isomer=L
SwapRes 40, Dt, Isomer=L
ShowAll
ColorMol Mol C,Red
ColorMol Mol D,Red
SaveSce (macrotarget)_A.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_A_water

#T
LoadSce (macrotarget).sce
SwapRes 1, DT, Isomer=L
SwapRes 2, DT, Isomer=L
SwapRes 3, DT, Isomer=L
SwapRes 4, DT, Isomer=L
SwapRes 5, DT, Isomer=L
SwapRes 6, DT, Isomer=L
SwapRes 7, DT, Isomer=L
SwapRes 8, DT, Isomer=L
SwapRes 9, DT, Isomer=L
SwapRes 10, DT, Isomer=L
SwapRes 11, DT, Isomer=L
SwapRes 12, DT, Isomer=L
SwapRes 13, DT, Isomer=L
SwapRes 14, DT, Isomer=L
SwapRes 15, DT, Isomer=L
SwapRes 16, DT, Isomer=L
SwapRes 17, DT, Isomer=L
SwapRes 18, DT, Isomer=L
SwapRes 19, DT, Isomer=L
SwapRes 20, DT, Isomer=L
SwapRes 21, Da, Isomer=L
SwapRes 22, Da, Isomer=L
SwapRes 23, Da, Isomer=L
SwapRes 24, Da, Isomer=L
SwapRes 25, Da, Isomer=L
SwapRes 26, Da, Isomer=L
SwapRes 27, Da, Isomer=L
SwapRes 28, Da, Isomer=L
SwapRes 29, Da, Isomer=L
SwapRes 30, Da, Isomer=L
SwapRes 31, Da, Isomer=L
SwapRes 32, Da, Isomer=L
SwapRes 33, Da, Isomer=L
SwapRes 34, Da, Isomer=L
SwapRes 35, Da, Isomer=L
SwapRes 36, Da, Isomer=L
SwapRes 37, Da, Isomer=L
SwapRes 38, Da, Isomer=L
SwapRes 39, Da, Isomer=L
SwapRes 40, Da, Isomer=L
ShowAll
ColorMol Mol C,Red
ColorMol Mol D,Red
SaveSce (macrotarget)_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_AT_water
#G
LoadSce (macrotarget).sce
SwapRes 1, DG, Isomer=L
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SwapRes 4, DG, Isomer=L
SwapRes 5, DG, Isomer=L
SwapRes 6, DG, Isomer=L
SwapRes 7, DG, Isomer=L
SwapRes 8, DG, Isomer=L
SwapRes 9, DG, Isomer=L
SwapRes 10, DG, Isomer=L
SwapRes 11, DG, Isomer=L
SwapRes 12, DG, Isomer=L
SwapRes 13, DG, Isomer=L
SwapRes 14, DG, Isomer=L
SwapRes 15, DG, Isomer=L
SwapRes 16, DG, Isomer=L
SwapRes 17, DG, Isomer=L
SwapRes 18, DG, Isomer=L
SwapRes 19, DG, Isomer=L
SwapRes 20, DG, Isomer=L
SwapRes 21, Dc, Isomer=L
SwapRes 22, Dc, Isomer=L
SwapRes 23, Dc, Isomer=L
SwapRes 24, Dc, Isomer=L
SwapRes 25, Dc, Isomer=L
SwapRes 26, Dc, Isomer=L
SwapRes 27, Dc, Isomer=L
SwapRes 28, Dc, Isomer=L
SwapRes 29, Dc, Isomer=L
SwapRes 30, Dc, Isomer=L
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SwapRes 33, Dc, Isomer=L
SwapRes 34, Dc, Isomer=L
SwapRes 35, Dc, Isomer=L
SwapRes 36, Dc, Isomer=L
SwapRes 37, Dc, Isomer=L
SwapRes 38, Dc, Isomer=L
SwapRes 39, Dc, Isomer=L
SwapRes 40, Dc, Isomer=L
ShowAll
ColorMol Mol C, Red
ColorMol Mol D, Red
SaveSce (macrotarget)_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_ATG_water

#C
LoadSce (macrotarget).sce
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SwapRes 6, DC, Isomer=L
SwapRes 7, DC, Isomer=L
SwapRes 8, DC, Isomer=L
SwapRes 9, DC, Isomer=L
SwapRes 10, DC, Isomer=L
SwapRes 11, DC, Isomer=L
SwapRes 12, DC, Isomer=L
SwapRes 13, DC, Isomer=L
SwapRes 14, DC, Isomer=L
SwapRes 15, DC, Isomer=L
SwapRes 16, DC, Isomer=L
SwapRes 17, DC, Isomer=L
SwapRes 18, DC, Isomer=L
SwapRes 19, DC, Isomer=L
SwapRes 20, DC, Isomer=L
SwapRes 21, Dg, Isomer=L
SwapRes 22, Dg, Isomer=L
SwapRes 23, Dg, Isomer=L
SwapRes 24, Dg, Isomer=L
SwapRes 25, Dg, Isomer=L
SwapRes 26, Dg, Isomer=L
SwapRes 27, Dg, Isomer=L
SwapRes 28, Dg, Isomer=L
SwapRes 29, Dg, Isomer=L
SwapRes 30, Dg, Isomer=L
SwapRes 31, Dg, Isomer=L
SwapRes 32, Dg, Isomer=L
SwapRes 33, Dg, Isomer=L
SwapRes 34, Dg, Isomer=L
SwapRes 35, Dg, Isomer=L
SwapRes 36, Dg, Isomer=L
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SwapRes 40, Dg, Isomer=L
ShowAll
ColorMol Mol C, Red
ColorMol Mol D, Red
SaveSce (macrotarget)_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_ATGC_water

#C1 on A array
LoadSce (macrotarget)_A.sce

SwapRes 1, (first), Isomer=L
SwapRes 2, (second), Isomer=L
SwapRes 3, (third), Isomer=L
SwapRes 4, (fourth), Isomer=L
SwapRes 5, (fifth), Isomer=L
SwapRes 6, (six), Isomer=L
SwapRes 35, (csix), Isomer=L
SwapRes 36, (cfifth), Isomer=L
SwapRes 37, (cfourth), Isomer=L
SwapRes 38, (cthird), Isomer=L
SwapRes 39, (csecond), Isomer=L
SwapRes 40, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C1_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C1_A_water.sce

#C2 on A array
LoadSce (macrotarget)_A.sce

SwapRes 2, (first), Isomer=L
SwapRes 3, (second), Isomer=L
SwapRes 4, (third), Isomer=L
SwapRes 5, (fourth), Isomer=L
SwapRes 6, (fifth), Isomer=L
SwapRes 7, (six), Isomer=L
SwapRes 34, (csix), Isomer=L
SwapRes 35, (cfifth), Isomer=L
SwapRes 36, (cfourth), Isomer=L
SwapRes 37, (cthird), Isomer=L
SwapRes 38, (csecond), Isomer=L
SwapRes 39, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C2_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C2_A_water.sce

#C3 on A array
LoadSce (macrotarget)_A.sce

SwapRes 3, (first), Isomer=L
SwapRes 4, (second), Isomer=L
SwapRes 5, (third), Isomer=L
SwapRes 6, (fourth), Isomer=L
SwapRes 7, (fifth), Isomer=L
SwapRes 8, (six), Isomer=L

SwapRes 33, (csix), Isomer=L
SwapRes 34, (cfifth), Isomer=L
SwapRes 35, (cfourth), Isomer=L
SwapRes 36, (cthird), Isomer=L
SwapRes 37, (csecond), Isomer=L
SwapRes 38, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C3_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C3_A_water.sce

#C4 on A array
LoadSce (macrotarget)_A.sce

SwapRes 4, (first), Isomer=L
SwapRes 5, (second), Isomer=L
SwapRes 6, (third), Isomer=L
SwapRes 7, (fourth), Isomer=L
SwapRes 8, (fifth), Isomer=L
SwapRes 9, (six), Isomer=L

SwapRes 32, (csix), Isomer=L
SwapRes 33, (cfifth), Isomer=L
SwapRes 34, (cfourth), Isomer=L
SwapRes 35, (cthird), Isomer=L
SwapRes 36, (csecond), Isomer=L
SwapRes 37, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C4_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C4_A_water.sce

#C5 on A array
LoadSce (macrotarget)_A.sce

SwapRes 5, (first), Isomer=L
SwapRes 6, (second), Isomer=L
SwapRes 7, (third), Isomer=L
SwapRes 8, (fourth), Isomer=L
SwapRes 9, (fifth), Isomer=L
SwapRes 10, (six), Isomer=L
SwapRes 31, (csix), Isomer=L
SwapRes 32, (cfifth), Isomer=L
SwapRes 33, (cfourth), Isomer=L
SwapRes 34, (cthird), Isomer=L
SwapRes 35, (csecond), Isomer=L
SwapRes 36, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C5_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C5_A_water.sce

#C6 on A array
LoadSce (macrotarget)_A.sce

SwapRes 6, (first), Isomer=L
SwapRes 7, (second), Isomer=L
SwapRes 8, (third), Isomer=L
SwapRes 9, (fourth), Isomer=L
SwapRes 10, (fifth), Isomer=L
SwapRes 11, (six), Isomer=L
SwapRes 30, (csix), Isomer=L
SwapRes 31, (cfifth), Isomer=L
SwapRes 32, (cfourth), Isomer=L
SwapRes 33, (cthird), Isomer=L
SwapRes 34, (csecond), Isomer=L
SwapRes 35, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C6_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C6_A_water.sce
#C7 on A array
LoadSce (macrotarget)_A.sce

SwapRes 7, (first), Isomer=L
SwapRes 8, (second), Isomer=L
SwapRes 9, (third), Isomer=L
SwapRes 10, (fourth), Isomer=L
SwapRes 11, (fifth), Isomer=L
SwapRes 12, (six), Isomer=L

SwapRes 29, (csix), Isomer=L
SwapRes 30, (cfifth), Isomer=L
SwapRes 31, (cfourth), Isomer=L
SwapRes 32, (cthird), Isomer=L
SwapRes 33, (csecond), Isomer=L
SwapRes 34, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C7_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C7_A_water.sce

#C8 on A array
LoadSce (macrotarget)_A.sce

SwapRes 8, (first), Isomer=L
SwapRes 9, (second), Isomer=L
SwapRes 10, (third), Isomer=L
SwapRes 11, (fourth), Isomer=L
SwapRes 12, (fifth), Isomer=L
SwapRes 13, (six), Isomer=L

SwapRes 28, (csix), Isomer=L
SwapRes 29, (cfifth), Isomer=L
SwapRes 30, (cfourth), Isomer=L
SwapRes 31, (cthird), Isomer=L
SwapRes 32, (csecond), Isomer=L
SwapRes 33, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C8_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C8_A_water.sce

#C9 on A array
LoadSce (macrotarget)_A.sce

SwapRes 9, (first), Isomer=L
SwapRes 10, (second), Isomer=L
SwapRes 11, (third), Isomer=L
SwapRes 12, (fourth), Isomer=L
SwapRes 13, (fifth), Isomer=L
SwapRes 14, (six), Isomer=L
SwapRes 27, (csix), Isomer=L
SwapRes 28, (cfifth), Isomer=L
SwapRes 29, (cfourth), Isomer=L
SwapRes 30, (cthird), Isomer=L
SwapRes 31, (csecond), Isomer=L
SwapRes 32, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget) _C9_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget) _C9_A_water.sce

#C10 on A array
LoadSce (macrotarget) _A.sce
SwapRes 10, (first), Isomer=L
SwapRes 11, (second), Isomer=L
SwapRes 12, (third), Isomer=L
SwapRes 13, (fourth), Isomer=L
SwapRes 14, (fifth), Isomer=L
SwapRes 15, (six), Isomer=L
SwapRes 26, (csix), Isomer=L
SwapRes 27, (cfifth), Isomer=L
SwapRes 28, (cfourth), Isomer=L
SwapRes 29, (cthird), Isomer=L
SwapRes 30, (csecond), Isomer=L
SwapRes 31, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget) _C10_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget) _C10_A_water.sce

#C11 on A array
LoadSce (macrotarget) _A.sce
SwapRes 11, (first), Isomer=L
SwapRes 12, (second), Isomer=L
SwapRes 13, (third), Isomer=L
SwapRes 14, (fourth), Isomer=L
SwapRes 15, (fifth), Isomer=L
SwapRes 16, (six), Isomer=L
SwapRes 25, (csix), Isomer=L
SwapRes 26, (cfifth), Isomer=L
SwapRes 27, (cfourth), Isomer=L
SwapRes 28, (cthird), Isomer=L
SwapRes 29, (csecond), Isomer=L
SwapRes 30, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C11_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C11_A_water.sce

#C12 on A array
LoadSce (macrotarget)_A.sce

SwapRes 12, (first), Isomer=L
SwapRes 13, (second), Isomer=L
SwapRes 14, (third), Isomer=L
SwapRes 15, (fourth), Isomer=L
SwapRes 16, (fifth), Isomer=L
SwapRes 17, (six), Isomer=L

SwapRes 24, (csix), Isomer=L
SwapRes 25, (cfifth), Isomer=L
SwapRes 26, (cfourth), Isomer=L
SwapRes 27, (cthird), Isomer=L
SwapRes 28, (csecond), Isomer=L
SwapRes 29, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C12_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C12_A_water.sce

#C13 on A array
LoadSce (macrotarget)_A.sce

SwapRes 13, (first), Isomer=L
SwapRes 14, (second), Isomer=L
SwapRes 15, (third), Isomer=L
SwapRes 16, (fourth), Isomer=L
SwapRes 17, (fifth), Isomer=L
SwapRes 18, (six), Isomer=L

SwapRes 23, (csix), Isomer=L
SwapRes 24, (cfifth), Isomer=L
SwapRes 25, (cfourth), Isomer=L
SwapRes 26, (cthird), Isomer=L
SwapRes 27, (csecond), Isomer=L
SwapRes 28, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C13_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C13_A_water.sce

#C14 on A array
LoadSce (macrotarget)_A.sce

SwapRes 14, (first), Isomer=L
SwapRes 15, (second), Isomer=L
SwapRes 16, (third), Isomer=L
SwapRes 17, (fourth), Isomer=L
SwapRes 18, (fifth), Isomer=L
SwapRes 19, (six), Isomer=L
SwapRes 22, (csix), Isomer=L
SwapRes 23, (cfifth), Isomer=L
SwapRes 24, (cfourth), Isomer=L
SwapRes 25, (cthird), Isomer=L
SwapRes 26, (csecond), Isomer=L
SwapRes 27, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C14_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C14_A_water.sce

#C15 on A array
LoadSce (macrotarget)_A.sce

SwapRes 15, (first), Isomer=L
SwapRes 16, (second), Isomer=L
SwapRes 17, (third), Isomer=L
SwapRes 18, (fourth), Isomer=L
SwapRes 19, (fifth), Isomer=L
SwapRes 20, (six), Isomer=L
SwapRes 21, (csix), Isomer=L
SwapRes 22, (cfifth), Isomer=L
SwapRes 23, (cfourth), Isomer=L
SwapRes 24, (cthird), Isomer=L
SwapRes 25, (csecond), Isomer=L
SwapRes 26, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C15_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C15_A_water.sce
#D21 on A array
LoadSce (macrotarget)_A.sce

SwapRes 21, (first), Isomer=L
SwapRes 22, (second), Isomer=L
SwapRes 23, (third), Isomer=L
SwapRes 24, (fourth), Isomer=L
SwapRes 25, (fifth), Isomer=L
SwapRes 26, (six), Isomer=L

SwapRes 20, (cfirst), Isomer=L
SwapRes 19, (csecond), Isomer=L
SwapRes 18, (cthird), Isomer=L
SwapRes 17, (cfourth), Isomer=L
SwapRes 16, (cfifth), Isomer=L
SwapRes 15, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D21_A.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D21_A_water.sce

#D22 on A array
LoadSce (macrotarget)_A.sce

SwapRes 22, (first), Isomer=L
SwapRes 23, (second), Isomer=L
SwapRes 24, (third), Isomer=L
SwapRes 25, (fourth), Isomer=L
SwapRes 26, (fifth), Isomer=L
SwapRes 27, (six), Isomer=L

SwapRes 19, (cfirst), Isomer=L
SwapRes 18, (csecond), Isomer=L
SwapRes 17, (cthird), Isomer=L
SwapRes 16, (cfourth), Isomer=L
SwapRes 15, (cfifth), Isomer=L
SwapRes 14, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D22_A.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D22_A_water.sce

#D23 on A array
LoadSce (macrotarget)_A.sce
SwapRes 23, (first), Isomer=L
SwapRes 24, (second), Isomer=L
SwapRes 25, (third), Isomer=L
SwapRes 26, (fourth), Isomer=L
SwapRes 27, (fifth), Isomer=L
SwapRes 28, (six), Isomer=L

SwapRes 18, (cfirst), Isomer=L
SwapRes 17, (csecond), Isomer=L
SwapRes 16, (cthird), Isomer=L
SwapRes 15, (cfourth), Isomer=L
SwapRes 14, (cfifth), Isomer=L
SwapRes 13, (csix), Isomer=L

ShowAll
SaveSce (macrotarget) _D23_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget) _D23_A_water.sce

#D24 on A array
LoadSce (macrotarget) _A.sce

SwapRes 24, (first), Isomer=L
SwapRes 25, (second), Isomer=L
SwapRes 26, (third), Isomer=L
SwapRes 27, (fourth), Isomer=L
SwapRes 28, (fifth), Isomer=L
SwapRes 29, (six), Isomer=L

SwapRes 17, (cfirst), Isomer=L
SwapRes 16, (csecond), Isomer=L
SwapRes 15, (cthird), Isomer=L
SwapRes 14, (cfourth), Isomer=L
SwapRes 13, (cfifth), Isomer=L
SwapRes 12, (csix), Isomer=L

ShowAll
SaveSce (macrotarget) _D24_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget) _D24_A_water.sce

#D25 on A array
LoadSce (macrotarget) _A.sce

SwapRes 25, (first), Isomer=L
SwapRes 26, (second), Isomer=L
SwapRes 27, (third), Isomer=L
SwapRes 28, (fourth), Isomer=L
SwapRes 29, (fifth), Isomer=L
SwapRes 30, (six), Isomer=L
SwapRes 16, (cfirst), Isomer=L
SwapRes 15, (csecond), Isomer=L
SwapRes 14, (cthird), Isomer=L
SwapRes 13, (cfourth), Isomer=L
SwapRes 12, (cfifth), Isomer=L
SwapRes 11, (csix), Isomer=L
ShowAll
SaveSce (macrotarget)_D25_A.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D25_A_water.sce

#D26 on A array
LoadSce (macrotarget)_A.sce

SwapRes 26, (first), Isomer=L
SwapRes 27, (second), Isomer=L
SwapRes 28, (third), Isomer=L
SwapRes 29, (fourth), Isomer=L
SwapRes 30, (fifth), Isomer=L
SwapRes 31, (six), Isomer=L
SwapRes 15, (cfirst), Isomer=L
SwapRes 14, (csecond), Isomer=L
SwapRes 13, (cthird), Isomer=L
SwapRes 12, (cfourth), Isomer=L
SwapRes 11, (cfifth), Isomer=L
SwapRes 10, (csix), Isomer=L
ShowAll
SaveSce (macrotarget)_D26_A.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D26_A_water.sce

#D27 on A array
LoadSce (macrotarget)_A.sce

SwapRes 27, (first), Isomer=L
SwapRes 28, (second), Isomer=L
SwapRes 29, (third), Isomer=L
SwapRes 30, (fourth), Isomer=L
SwapRes 31, (fifth), Isomer=L
SwapRes 32, (six), Isomer=L
SwapRes 14, (cfirst), Isomer=L
SwapRes 13, (csecond), Isomer=L
SwapRes 12, (cthird), Isomer=L
SwapRes 11, (cfourth), Isomer=L
SwapRes 10, (cfifth), Isomer=L
SwapRes 9, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D27_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D27_A_water.sce

#D28 on A array
LoadSce (macrotarget)_A.sce

SwapRes 28, (first), Isomer=L
SwapRes 29, (second), Isomer=L
SwapRes 30, (third), Isomer=L
SwapRes 31, (fourth), Isomer=L
SwapRes 32, (fifth), Isomer=L
SwapRes 33, (six), Isomer=L

SwapRes 13, (cfirst), Isomer=L
SwapRes 12, (csecond), Isomer=L
SwapRes 11, (cthird), Isomer=L
SwapRes 10, (cfourth), Isomer=L
SwapRes 9, (cfifth), Isomer=L
SwapRes 8, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D28_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D28_A_water.sce

#D29 on A array
LoadSce (macrotarget)_A.sce

SwapRes 29, (first), Isomer=L
SwapRes 30, (second), Isomer=L
SwapRes 31, (third), Isomer=L
SwapRes 32, (fourth), Isomer=L
SwapRes 33, (fifth), Isomer=L
SwapRes 34, (six), Isomer=L

SwapRes 12, (cfirst), Isomer=L
SwapRes 11, (csecond), Isomer=L
SwapRes 10, (cthird), Isomer=L
SwapRes 9, (cfourth), Isomer=L
SwapRes 8, (cfifth), Isomer=L
SwapRes 7, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D29_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D29_A_water.sce

#D30 on A array
LoadSce (macrotarget)_A.sce

SwapRes 30, (first), Isomer=L
SwapRes 31, (second), Isomer=L
SwapRes 32, (third), Isomer=L
SwapRes 33, (fourth), Isomer=L
SwapRes 34, (fifth), Isomer=L
SwapRes 35, (six), Isomer=L

SwapRes 11, (cfirst), Isomer=L
SwapRes 10, (csecond), Isomer=L
SwapRes 9, (cthird), Isomer=L
SwapRes 8, (cfourth), Isomer=L
SwapRes 7, (cfifth), Isomer=L
SwapRes 6, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D30_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D30_A_water.sce

#D31 on A array
LoadSce (macrotarget)_A.sce

SwapRes 31, (first), Isomer=L
SwapRes 32, (second), Isomer=L
SwapRes 33, (third), Isomer=L
SwapRes 34, (fourth), Isomer=L
SwapRes 35, (fifth), Isomer=L
SwapRes 36, (six), Isomer=L

SwapRes 10, (cfirst), Isomer=L
SwapRes 9, (csecond), Isomer=L
SwapRes 8, (cthird), Isomer=L
SwapRes 7, (cfourth), Isomer=L
SwapRes 6, (cfifth), Isomer=L
SwapRes 5, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D31_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D31_A_water.sce

#D32 on A array
LoadSce (macrotarget)_A.sce
SwapRes 32, (first), Isomer=L
SwapRes 33, (second), Isomer=L
SwapRes 34, (third), Isomer=L
SwapRes 35, (fourth), Isomer=L
SwapRes 36, (fifth), Isomer=L
SwapRes 37, (six), Isomer=L
SwapRes 38, (cfirst), Isomer=L
SwapRes 39, (csecond), Isomer=L
SwapRes 39, (cthird), Isomer=L
SwapRes 39, (cfourth), Isomer=L
SwapRes 39, (cfifth), Isomer=L
SwapRes 39, (csix), Isomer=L
ShowAll
SaveSce (macrotarget)_D32_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D32_A_water.sce

#D33 on A array
LoadSce (macrotarget)_A.sce
SwapRes 33, (first), Isomer=L
SwapRes 34, (second), Isomer=L
SwapRes 35, (third), Isomer=L
SwapRes 36, (fourth), Isomer=L
SwapRes 37, (fifth), Isomer=L
SwapRes 38, (six), Isomer=L
SwapRes 38, (cfirst), Isomer=L
SwapRes 39, (csecond), Isomer=L
SwapRes 39, (cthird), Isomer=L
SwapRes 39, (cfourth), Isomer=L
SwapRes 39, (cfifth), Isomer=L
SwapRes 39, (csix), Isomer=L
ShowAll
SaveSce (macrotarget)_D33_A.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D33_A_water.sce

#D34 on A array
LoadSce (macrotarget)_A.sce
SwapRes 34, (first), Isomer=L
SwapRes 35, (second), Isomer=L
SwapRes 36, (third), Isomer=L
SwapRes 37, (fourth), Isomer=L
SwapRes 38, (fifth), Isomer=L
SwapRes 39, (six), Isomer=L
SwapRes 7, (cfirst), Isomer=L
SwapRes 6, (csecond), Isomer=L
SwapRes 5, (cthird), Isomer=L
SwapRes 4, (cfourth), Isomer=L
SwapRes 3, (cfifth), Isomer=L
SwapRes 2, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D34_A.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D34_A_water.sce

#D35 on A array
LoadSce (macrotarget)_A.sce

SwapRes 35, (first), Isomer=L
SwapRes 36, (second), Isomer=L
SwapRes 37, (third), Isomer=L
SwapRes 38, (fourth), Isomer=L
SwapRes 39, (fifth), Isomer=L
SwapRes 40, (six), Isomer=L

SwapRes 6, (cfirst), Isomer=L
SwapRes 5, (csecond), Isomer=L
SwapRes 4, (cthird), Isomer=L
SwapRes 3, (cfourth), Isomer=L
SwapRes 2, (cfifth), Isomer=L
SwapRes 1, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D35_A.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D35_A_water.sce

#C1 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 1, (first), Isomer=L
SwapRes 2, (second), Isomer=L
SwapRes 3, (third), Isomer=L
SwapRes 4, (fourth), Isomer=L
SwapRes 5, (fifth), Isomer=L
SwapRes 6, (six), Isomer=L

SwapRes 35, (csix), Isomer=L
SwapRes 36, (cfifth), Isomer=L
SwapRes 37, (cfourth), Isomer=L
SwapRes 38, (cthird), Isomer=L
SwapRes 39, (csecond), Isomer=L
SwapRes 40, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C1_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C1_AT_water.sce

#C2 on T array
LoadSce (macrotarget)_AT.sce
SwapRes 2, (first), Isomer=L
SwapRes 3, (second), Isomer=L
SwapRes 4, (third), Isomer=L
SwapRes 5, (fourth), Isomer=L
SwapRes 6, (fifth), Isomer=L
SwapRes 7, (six), Isomer=L
SwapRes 34, (csix), Isomer=L
SwapRes 35, (cfifth), Isomer=L
SwapRes 36, (cfourth), Isomer=L
SwapRes 37, (cthird), Isomer=L
SwapRes 38, (csecond), Isomer=L
SwapRes 39, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C2_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C2_AT_water.sce

#C3 on T array
LoadSce (macrotarget)_AT.sce
SwapRes 3, (first), Isomer=L
SwapRes 4, (second), Isomer=L
SwapRes 5, (third), Isomer=L
SwapRes 6, (fourth), Isomer=L
SwapRes 7, (fifth), Isomer=L
SwapRes 8, (six), Isomer=L
SwapRes 33, (csix), Isomer=L
SwapRes 34, (cfifth), Isomer=L
SwapRes 35, (cfourth), Isomer=L
SwapRes 36, (cthird), Isomer=L
SwapRes 37, (csecond), Isomer=L
SwapRes 38, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C3_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
Switch Obj 3, off
SaveSce (macrotarget)_C3_AT_water.sce

#C4 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 4, (first), Isomer=L
SwapRes 5, (second), Isomer=L
SwapRes 6, (third), Isomer=L
SwapRes 7, (fourth), Isomer=L
SwapRes 8, (fifth), Isomer=L
SwapRes 9, (six), Isomer=L

SwapRes 32, (csix), Isomer=L
SwapRes 33, (cfifth), Isomer=L
SwapRes 34, (cfourth), Isomer=L
SwapRes 35, (cthird), Isomer=L
SwapRes 36, (csecond), Isomer=L
SwapRes 37, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C4_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
Switch Obj 3, off
SaveSce (macrotarget)_C4_AT_water.sce

#C5 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 5, (first), Isomer=L
SwapRes 6, (second), Isomer=L
SwapRes 7, (third), Isomer=L
SwapRes 8, (fourth), Isomer=L
SwapRes 9, (fifth), Isomer=L
SwapRes 10, (six), Isomer=L

SwapRes 31, (csix), Isomer=L
SwapRes 32, (cfifth), Isomer=L
SwapRes 33, (cfourth), Isomer=L
SwapRes 34, (cthird), Isomer=L
SwapRes 35, (csecond), Isomer=L
SwapRes 36, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C5_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
Switch Obj 3, off
SaveSce (macrotarget)_C5_AT_water.sce

#C6 on T array
LoadSce (macrotarget)_AT.sce
SwapRes 6, (first), Isomer=L
SwapRes 7, (second), Isomer=L
SwapRes 8, (third), Isomer=L
SwapRes 9, (fourth), Isomer=L
SwapRes 10, (fifth), Isomer=L
SwapRes 11, (six), Isomer=L

SwapRes 30, (csix), Isomer=L
SwapRes 31, (cfifth), Isomer=L
SwapRes 32, (cfourth), Isomer=L
SwapRes 33, (cthird), Isomer=L
SwapRes 34, (csecond), Isomer=L
SwapRes 35, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C6_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C6_AT_water.sce

#C7 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 7, (first), Isomer=L
SwapRes 8, (second), Isomer=L
SwapRes 9, (third), Isomer=L
SwapRes 10, (fourth), Isomer=L
SwapRes 11, (fifth), Isomer=L
SwapRes 12, (six), Isomer=L

SwapRes 29, (csix), Isomer=L
SwapRes 30, (cfifth), Isomer=L
SwapRes 31, (cfourth), Isomer=L
SwapRes 32, (cthird), Isomer=L
SwapRes 33, (csecond), Isomer=L
SwapRes 34, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C7_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C7_AT_water.sce

#C8 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 8, (first), Isomer=L
SwapRes 9, (second), Isomer=L
SwapRes 10, (third), Isomer=L
SwapRes 11, (fourth), Isomer=L
SwapRes 12, (fifth), Isomer=L
SwapRes 13, (six), Isomer=L
SwapRes 28, (csix), Isomer=L
SwapRes 29, (cfifth), Isomer=L
SwapRes 30, (cfourth), Isomer=L
SwapRes 31, (cthird), Isomer=L
SwapRes 32, (csecond), Isomer=L
SwapRes 33, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C8_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C8_AT_water.sce

#C9 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 9, (first), Isomer=L
SwapRes 10, (second), Isomer=L
SwapRes 11, (third), Isomer=L
SwapRes 12, (fourth), Isomer=L
SwapRes 13, (fifth), Isomer=L
SwapRes 14, (six), Isomer=L
SwapRes 27, (csix), Isomer=L
SwapRes 28, (cfifth), Isomer=L
SwapRes 29, (cfourth), Isomer=L
SwapRes 30, (cthird), Isomer=L
SwapRes 31, (csecond), Isomer=L
SwapRes 32, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C9_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C9_AT_water.sce

#C10 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 10, (first), Isomer=L
SwapRes 11, (second), Isomer=L
SwapRes 12, (third), Isomer=L
SwapRes 13, (fourth), Isomer=L
SwapRes 14, (fifth), Isomer=L
SwapRes 15, (six), Isomer=L
SwapRes 26, (csix), Isomer=L
SwapRes 27, (cfifth), Isomer=L
SwapRes 28, (cfourth), Isomer=L
SwapRes 29, (cthird), Isomer=L
SwapRes 30, (csecond), Isomer=L
SwapRes 31, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C10_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C10_AT_water.sce

#C11 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 11, (first), Isomer=L
SwapRes 12, (second), Isomer=L
SwapRes 13, (third), Isomer=L
SwapRes 14, (fourth), Isomer=L
SwapRes 15, (fifth), Isomer=L
SwapRes 16, (six), Isomer=L
SwapRes 24, (csix), Isomer=L
SwapRes 25, (cfifth), Isomer=L
SwapRes 26, (cfourth), Isomer=L
SwapRes 27, (cthird), Isomer=L
SwapRes 28, (csecond), Isomer=L
SwapRes 29, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C11_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C11_AT_water.sce

#C12 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 12, (first), Isomer=L
SwapRes 13, (second), Isomer=L
SwapRes 14, (third), Isomer=L
SwapRes 15, (fourth), Isomer=L
SwapRes 16, (fifth), Isomer=L
SwapRes 17, (six), Isomer=L
SwapRes 25, (csix), Isomer=L
SwapRes 26, (cfifth), Isomer=L
SwapRes 27, (cfourth), Isomer=L
SwapRes 28, (cthird), Isomer=L
SwapRes 29, (csecond), Isomer=L
SwapRes 30, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C12_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C12_AT_water.sce

#C13 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 13, (first), Isomer=L
SwapRes 14, (second), Isomer=L
SwapRes 15, (third), Isomer=L
SwapRes 16, (fourth), Isomer=L
SwapRes 17, (fifth), Isomer=L
SwapRes 18, (six), Isomer=L
SwapRes 23, (csix), Isomer=L
SwapRes 24, (cfifth), Isomer=L
SwapRes 25, (cfourth), Isomer=L
SwapRes 26, (cthird), Isomer=L
SwapRes 27, (csecond), Isomer=L
SwapRes 28, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C13_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C13_AT_water.sce

#C14 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 14, (first), Isomer=L
SwapRes 15, (second), Isomer=L
SwapRes 16, (third), Isomer=L
SwapRes 17, (fourth), Isomer=L
SwapRes 18, (fifth), Isomer=L
SwapRes 19, (six), Isomer=L
SwapRes 22, (csix), Isomer=L
SwapRes 23, (cfifth), Isomer=L
SwapRes 24, (cfourth), Isomer=L
SwapRes 25, (cthird), Isomer=L
SwapRes 26, (csecond), Isomer=L
SwapRes 27, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C14_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C14_AT_water.sce

#C15 on T array
LoadSce (macrotarget)_AT.sce
SwapRes 15, (first), Isomer=L
SwapRes 16, (second), Isomer=L
SwapRes 17, (third), Isomer=L
SwapRes 18, (fourth), Isomer=L
SwapRes 19, (fifth), Isomer=L
SwapRes 20, (six), Isomer=L
SwapRes 21, (csix), Isomer=L
SwapRes 22, (cfirst), Isomer=L
SwapRes 23, (csecond), Isomer=L
SwapRes 24, (cthird), Isomer=L
SwapRes 25, (cfourth), Isomer=L
SwapRes 26, (cfifth), Isomer=L

ShowAll
SaveSce (macrotarget)_C15_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C15_AT_water.sce

#D21 on T array
LoadSce (macrotarget)_AT.sce
SWAPRES 21, (first), Isomer=L
SWAPRES 22, (second), Isomer=L
SWAPRES 23, (third), Isomer=L
SWAPRES 24, (fourth), Isomer=L
SWAPRES 25, (fifth), Isomer=L
SWAPRES 26, (six), Isomer=L
SWAPRES 20, (cfirst), Isomer=L
SWAPRES 19, (csecond), Isomer=L
SWAPRES 18, (cthird), Isomer=L
SWAPRES 17, (cfourth), Isomer=L
SWAPRES 16, (cfifth), Isomer=L
SWAPRES 15, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D21_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D21_AT_water.sce

#D22 on T array
LoadSce (macrotarget)_AT.sce
SWAPRES 22, (first), Isomer=L
SWAPRES 23, (second), Isomer=L
SWAPRES 24, (third), Isomer=L
SwapRes 25, (fourth), Isomer=L
SwapRes 26, (fifth), Isomer=L
SwapRes 27, (six), Isomer=L

SwapRes 19, (cfirst), Isomer=L
SwapRes 18, (csecond), Isomer=L
SwapRes 17, (cthird), Isomer=L
SwapRes 16, (cfourth), Isomer=L
SwapRes 15, (cfifth), Isomer=L
SwapRes 14, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D22_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D22_AT_water.sce

#D23 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 23, (first), Isomer=L
SwapRes 24, (second), Isomer=L
SwapRes 25, (third), Isomer=L
SwapRes 26, (fourth), Isomer=L
SwapRes 27, (fifth), Isomer=L
SwapRes 28, (six), Isomer=L

SwapRes 18, (cfirst), Isomer=L
SwapRes 17, (csecond), Isomer=L
SwapRes 16, (cthird), Isomer=L
SwapRes 15, (cfourth), Isomer=L
SwapRes 14, (cfifth), Isomer=L
SwapRes 13, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D23_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macro target)_D23_AT_water.sce

#D24 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 24, (first), Isomer=L
SwapRes 25, (second), Isomer=L
SwapRes 26, (third), Isomer=L
SwapRes 27, (fourth), Isomer=L
SwapRes 28, (fifth), Isomer=L
SwapRes 29, (six), Isomer=L

SwapRes 17, (cfirst), Isomer=L
SwapRes 16, (csecond), Isomer=L
SwapRes 15, (cthird), Isomer=L
SwapRes 14, (cfourth), Isomer=L
SwapRes 13, (cfifth), Isomer=L
SwapRes 12, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D24_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D24_AT_water.sce

#D25 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 25, (first), Isomer=L
SwapRes 26, (second), Isomer=L
SwapRes 27, (third), Isomer=L
SwapRes 28, (fourth), Isomer=L
SwapRes 29, (fifth), Isomer=L
SwapRes 30, (six), Isomer=L

SwapRes 16, (cfirst), Isomer=L
SwapRes 15, (csecond), Isomer=L
SwapRes 14, (cthird), Isomer=L
SwapRes 13, (cfourth), Isomer=L
SwapRes 12, (cfifth), Isomer=L
SwapRes 11, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D25_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D25_AT_water.sce

#D26 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 26, (first), Isomer=L
SwapRes 27, (second), Isomer=L
SwapRes 28, (third), Isomer=L
SwapRes 29, (fourth), Isomer=L
SwapRes 30, (fifth), Isomer=L
SwapRes 31, (six), Isomer=L

SwapRes 15, (cfirst), Isomer=L
SwapRes 14, (csecond), Isomer=L
SwapRes 13, (cthird), Isomer=L
SwapRes 12, (cfourth), Isomer=L
SwapRes 11, (cfifth), Isomer=L
SwapRes 10, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D26_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D26_AT_water.sce

#D27 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 27, (first), Isomer=L
SwapRes 28, (second), Isomer=L
SwapRes 29, (third), Isomer=L
SwapRes 30, (fourth), Isomer=L
SwapRes 31, (fifth), Isomer=L
SwapRes 32, (six), Isomer=L

SwapRes 14, (cfirst), Isomer=L
SwapRes 13, (csecond), Isomer=L
SwapRes 12, (cthird), Isomer=L
SwapRes 11, (cfourth), Isomer=L
SwapRes 10, (cfifth), Isomer=L
SwapRes 9, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D27_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D27_AT_water.sce

#D28 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 28, (first), Isomer=L
SwapRes 29, (second), Isomer=L
SwapRes 30, (third), Isomer=L
SwapRes 31, (fourth), Isomer=L
SwapRes 32, (fifth), Isomer=L
SwapRes 33, (six), Isomer=L

SwapRes 13, (cfirst), Isomer=L
SwapRes 12, (csecond), Isomer=L
SwapRes 11, (cthird), Isomer=L
SwapRes 10, (cfourth), Isomer=L
SwapRes 9, (cfifth), Isomer=L
SwapRes 8, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D28_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D28_AT_water.sce
#D29 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 29, (first), Isomer=L
SwapRes 30, (second), Isomer=L
SwapRes 31, (third), Isomer=L
SwapRes 32, (fourth), Isomer=L
SwapRes 33, (fifth), Isomer=L
SwapRes 34, (six), Isomer=L

SwapRes 12, (cfirst), Isomer=L
SwapRes 11, (csecond), Isomer=L
SwapRes 10, (cthird), Isomer=L
SwapRes 9, (cfourth), Isomer=L
SwapRes 8, (cfifth), Isomer=L
SwapRes 7, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D29_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D29_AT_water.sce

#D30 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 30, (first), Isomer=L
SwapRes 31, (second), Isomer=L
SwapRes 32, (third), Isomer=L
SwapRes 33, (fourth), Isomer=L
SwapRes 34, (fifth), Isomer=L
SwapRes 35, (six), Isomer=L

SwapRes 11, (cfirst), Isomer=L
SwapRes 10, (csecond), Isomer=L
SwapRes 9, (cthird), Isomer=L
SwapRes 8, (cfourth), Isomer=L
SwapRes 7, (cfifth), Isomer=L
SwapRes 6, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D30_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D30_AT_water.sce

#D31 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 31, (first), Isomer=L
SwapRes 32, (second), Isomer=L
SwapRes 33, (third), Isomer=L
SwapRes 34, (fourth), Isomer=L
SwapRes 35, (fifth), Isomer=L
SwapRes 36, (six), Isomer=L

SwapRes 10, (cfirst), Isomer=L
SwapRes 9, (csecond), Isomer=L
SwapRes 8, (cthird), Isomer=L
SwapRes 7, (cfourth), Isomer=L
SwapRes 6, (cfifth), Isomer=L
SwapRes 5, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D31_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D31_AT_water.sce

#D32 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 32, (first), Isomer=L
SwapRes 33, (second), Isomer=L
SwapRes 34, (third), Isomer=L
SwapRes 35, (fourth), Isomer=L
SwapRes 36, (fifth), Isomer=L
SwapRes 37, (six), Isomer=L

SwapRes 9, (cfirst), Isomer=L
SwapRes 8, (csecond), Isomer=L
SwapRes 7, (cthird), Isomer=L
SwapRes 6, (cfourth), Isomer=L
SwapRes 5, (cfifth), Isomer=L
SwapRes 4, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D32_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D32_AT_water.sce

#D33 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 33, (first), Isomer=L
SwapRes 34, (second), Isomer=L
SwapRes 35, (third), Isomer=L
SwapRes 36, (fourth), Isomer=L
SwapRes 37, (fifth), Isomer=L
SwapRes 38, (six), Isomer=L

SwapRes 8, (cfirst), Isomer=L
SwapRes 7, (csecond), Isomer=L
SwapRes 6, (cthird), Isomer=L
SwapRes 5, (cfourth), Isomer=L
SwapRes 4, (cfifth), Isomer=L
SwapRes 3, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D33_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D33_AT_water.sce

#D34 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 34, (first), Isomer=L
SwapRes 35, (second), Isomer=L
SwapRes 36, (third), Isomer=L
SwapRes 37, (fourth), Isomer=L
SwapRes 38, (fifth), Isomer=L
SwapRes 39, (six), Isomer=L

SwapRes 7, (cfirst), Isomer=L
SwapRes 6, (csecond), Isomer=L
SwapRes 5, (cthird), Isomer=L
SwapRes 4, (cfourth), Isomer=L
SwapRes 3, (cfifth), Isomer=L
SwapRes 2, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D34_AT.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D34_AT_water.sce

#D35 on T array
LoadSce (macrotarget)_AT.sce

SwapRes 35, (first), Isomer=L
SwapRes 36, (second), Isomer=L
SwapRes 37, (third), Isomer=L
SwapRes 38, (fourth), Isomer=L
SwapRes 39, (fifth), Isomer=L
SwapRes 40, (six), Isomer=L

SwapRes 6, (cfirst), Isomer=L
SwapRes 5, (csecond), Isomer=L
SwapRes 4, (cthird), Isomer=L
SwapRes 3, (cfourth), Isomer=L
SwapRes 2, (cfifth), Isomer=L
SwapRes 1, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D35_AT.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D35_AT_water.sce

#C1 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 1, (first), Isomer=L
SwapRes 2, (second), Isomer=L
SwapRes 3, (third), Isomer=L
SwapRes 4, (fourth), Isomer=L
SwapRes 5, (fifth), Isomer=L
SwapRes 6, (six), Isomer=L
SwapRes 35, (csix), Isomer=L
SwapRes 36, (cfifth), Isomer=L
SwapRes 37, (cfourth), Isomer=L
SwapRes 38, (cthird), Isomer=L
SwapRes 39, (csecond), Isomer=L
SwapRes 40, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C1_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C1_ATG_water.sce

#C2 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 2, (first), Isomer=L
SwapRes 3, (second), Isomer=L
SwapRes 4, (third), Isomer=L
SwapRes 5, (fourth), Isomer=L
SwapRes 6, (fifth), Isomer=L
SwapRes 7, (six), Isomer=L
SwapRes 34, (csix), Isomer=L
SwapRes 35, (cfifth), Isomer=L
SwapRes 36, (cfourth), Isomer=L
SwapRes 37, (cthird), Isomer=L
SwapRes 38, (csecond), Isomer=L
SwapRes 39, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C2_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C2_ATG_water.sce
#C3 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 3, (first), Isomer=L
SwapRes 4, (second), Isomer=L
SwapRes 5, (third), Isomer=L
SwapRes 6, (fourth), Isomer=L
SwapRes 7, (fifth), Isomer=L
SwapRes 8, (six), Isomer=L
SwapRes 33, (csix), Isomer=L
SwapRes 34, (cfifth), Isomer=L
SwapRes 35, (cfourth), Isomer=L
SwapRes 36, (cthird), Isomer=L
SwapRes 37, (csecond), Isomer=L
SwapRes 38, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C3_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C3_ATG_water.sce

#C4 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 4, (first), Isomer=L
SwapRes 5, (second), Isomer=L
SwapRes 6, (third), Isomer=L
SwapRes 7, (fourth), Isomer=L
SwapRes 8, (fifth), Isomer=L
SwapRes 9, (six), Isomer=L
SwapRes 32, (csix), Isomer=L
SwapRes 33, (cfifth), Isomer=L
SwapRes 34, (cfourth), Isomer=L
SwapRes 35, (cthird), Isomer=L
SwapRes 36, (csecond), Isomer=L
SwapRes 37, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C4_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C4_ATG_water.sce

#C5 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 5, (first), Isomer=L
SwapRes 6, (second), Isomer=L
SwapRes 7, (third), Isomer=L
SwapRes 8, (fourth), Isomer=L
SwapRes 9, (fifth), Isomer=L
SwapRes 10, (six), Isomer=L
SwapRes 31, (csix), Isomer=L
SwapRes 32, (cfifth), Isomer=L
SwapRes 33, (cfourth), Isomer=L
SwapRes 34, (cthird), Isomer=L
SwapRes 35, (csecond), Isomer=L
SwapRes 36, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C5_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C5_ATG_water.sce

#C6 on G array
LoadSce (macrotarget)_ATG.sce
SwapRes 6, (first), Isomer=L
SwapRes 7, (second), Isomer=L
SwapRes 8, (third), Isomer=L
SwapRes 9, (fourth), Isomer=L
SwapRes 10, (fifth), Isomer=L
SwapRes 11, (six), Isomer=L
SwapRes 30, (csix), Isomer=L
SwapRes 31, (cfifth), Isomer=L
SwapRes 32, (cfourth), Isomer=L
SwapRes 33, (cthird), Isomer=L
SwapRes 34, (csecond), Isomer=L
SwapRes 35, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C6_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C6_ATG_water.sce

#C7 on G array
LoadSce (macrotarget)_ATG.sce
SwapRes 7, (first), Isomer=L
SwapRes 8, (second), Isomer=L
SwapRes 9, (third), Isomer=L
SwapRes 10, (fourth), Isomer=L
SwapRes 11, (fifth), Isomer=L
SwapRes 12, (six), Isomer=L
SwapRes 29, (csix), Isomer=L
SwapRes 30, (cfifth), Isomer=L
SwapRes 31, (cfourth), Isomer=L
SwapRes 32, (cthird), Isomer=L
SwapRes 33, (csecond), Isomer=L
SwapRes 34, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C7_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C7_ATG_water.sce

#C8 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 8, (first), Isomer=L
SwapRes 9, (second), Isomer=L
SwapRes 10, (third), Isomer=L
SwapRes 11, (fourth), Isomer=L
SwapRes 12, (fifth), Isomer=L
SwapRes 13, (six), Isomer=L

SwapRes 28, (csix), Isomer=L
SwapRes 29, (cfifth), Isomer=L
SwapRes 30, (cfourth), Isomer=L
SwapRes 31, (cthird), Isomer=L
SwapRes 32, (csecond), Isomer=L
SwapRes 33, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C8_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C8_ATG_water.sce

#C9 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 9, (first), Isomer=L
SwapRes 10, (second), Isomer=L
SwapRes 11, (third), Isomer=L
SwapRes 12, (fourth), Isomer=L
SwapRes 13, (fifth), Isomer=L
SwapRes 14, (six), Isomer=L

SwapRes 27, (csix), Isomer=L
SwapRes 28, (cfifth), Isomer=L
SwapRes 29, (cfourth), Isomer=L
SwapRes 30, (cthird), Isomer=L
SwapRes 31, (csecond), Isomer=L
SwapRes 32, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C9_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C9_ATG_water.sce

#C10 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 10, (first), Isomer=L
SwapRes 11, (second), Isomer=L
SwapRes 12, (third), Isomer=L
SwapRes 13, (fourth), Isomer=L
SwapRes 14, (fifth), Isomer=L
SwapRes 15, (six), Isomer=L
SwapRes 26, (csix), Isomer=L
SwapRes 27, (cfifth), Isomer=L
SwapRes 28, (cfourth), Isomer=L
SwapRes 29, (cthird), Isomer=L
SwapRes 30, (csecond), Isomer=L
SwapRes 31, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C10_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C10_ATG_water.sce

#C11 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 11, (first), Isomer=L
SwapRes 12, (second), Isomer=L
SwapRes 13, (third), Isomer=L
SwapRes 14, (fourth), Isomer=L
SwapRes 15, (fifth), Isomer=L
SwapRes 16, (six), Isomer=L
SwapRes 25, (csix), Isomer=L
SwapRes 26, (cfifth), Isomer=L
SwapRes 27, (cfourth), Isomer=L
SwapRes 28, (cthird), Isomer=L
SwapRes 29, (csecond), Isomer=L
SwapRes 30, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C11_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C11_ATG_water.sce
#C12 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 12, (first), Isomer=L
SwapRes 13, (second), Isomer=L
SwapRes 14, (third), Isomer=L
SwapRes 15, (fourth), Isomer=L
SwapRes 16, (fifth), Isomer=L
SwapRes 17, (six), Isomer=L

SwapRes 24, (csix), Isomer=L
SwapRes 25, (cfifth), Isomer=L
SwapRes 26, (cfourth), Isomer=L
SwapRes 27, (cthird), Isomer=L
SwapRes 28, (csecond), Isomer=L
SwapRes 29, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C12_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C13_ATG_water.sce

#C13 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 13, (first), Isomer=L
SwapRes 14, (second), Isomer=L
SwapRes 15, (third), Isomer=L
SwapRes 16, (fourth), Isomer=L
SwapRes 17, (fifth), Isomer=L
SwapRes 18, (six), Isomer=L

SwapRes 23, (csix), Isomer=L
SwapRes 24, (cfifth), Isomer=L
SwapRes 25, (cfourth), Isomer=L
SwapRes 26, (cthird), Isomer=L
SwapRes 27, (csecond), Isomer=L
SwapRes 28, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C13_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_C13_ATG_water.sce

#C14 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 14, (first), Isomer=L
SwapRes 15, (second), Isomer=L
SwapRes 16, (third), Isomer=L  
SwapRes 17, (fourth), Isomer=L  
SwapRes 18, (fifth), Isomer=L  
SwapRes 19, (six), Isomer=L  

SwapRes 22, (csix), Isomer=L  
SwapRes 23, (cfifth), Isomer=L  
SwapRes 24, (cfourth), Isomer=L  
SwapRes 25, (cthird), Isomer=L  
SwapRes 26, (csecond), Isomer=L  
SwapRes 27, (cfirst), Isomer=L  

ShowAll  
SaveSce (macrotarget)_C14_ATG.sce  
CleanAll  
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0  
SwitchObj 3, off  
SaveSce (macrotarget)_C14_ATG_water.sce  

#C15 on G array  
LoadSce (macrotarget)_ATG.sce  

SwapRes 15, (first), Isomer=L  
SwapRes 16, (second), Isomer=L  
SwapRes 17, (third), Isomer=L  
SwapRes 18, (fourth), Isomer=L  
SwapRes 19, (fifth), Isomer=L  
SwapRes 20, (six), Isomer=L  

SwapRes 21, (csix), Isomer=L  
SwapRes 22, (cfifth), Isomer=L  
SwapRes 23, (cfourth), Isomer=L  
SwapRes 24, (cthird), Isomer=L  
SwapRes 25, (csecond), Isomer=L  
SwapRes 26, (cfirst), Isomer=L  

ShowAll  
SaveSce (macrotarget)_C15_ATG.sce  
CleanAll  
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0  
SwitchObj 3, off  
SaveSce (macrotarget)_C15_ATG_water.sce  

#D21 on G array  
LoadSce (macrotarget)_ATG.sce  

SwapRes 21, (first), Isomer=L  
SwapRes 22, (second), Isomer=L  
SwapRes 23, (third), Isomer=L  
SwapRes 24, (fourth), Isomer=L  
SwapRes 25, (fifth), Isomer=L  
SwapRes 26, (six), Isomer=L
SwapRes 20, (cfirst), Isomer=L
SwapRes 19, (csecond), Isomer=L
SwapRes 18, (cthird), Isomer=L
SwapRes 17, (cfourth), Isomer=L
SwapRes 16, (cfifth), Isomer=L
SwapRes 15, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D21_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D21_ATG_water.sce

#D22 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 22, (first), Isomer=L
SwapRes 23, (second), Isomer=L
SwapRes 24, (third), Isomer=L
SwapRes 25, (fourth), Isomer=L
SwapRes 26, (fifth), Isomer=L
SwapRes 27, (six), Isomer=L
SwapRes 19, (cfirst), Isomer=L
SwapRes 18, (csecond), Isomer=L
SwapRes 17, (cthird), Isomer=L
SwapRes 16, (cfourth), Isomer=L
SwapRes 15, (cfifth), Isomer=L
SwapRes 14, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D22_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D22_ATG_water.sce

#D23 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 23, (first), Isomer=L
SwapRes 24, (second), Isomer=L
SwapRes 25, (third), Isomer=L
SwapRes 26, (fourth), Isomer=L
SwapRes 27, (fifth), Isomer=L
SwapRes 28, (six), Isomer=L
SwapRes 18, (cfirst), Isomer=L
SwapRes 17, (csecond), Isomer=L
SwapRes 16, (cthird), Isomer=L
SwapRes 15, (cfourth), Isomer=L
SwapRes 14, (cfifth), Isomer=L
SwapRes 13, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D23_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D23_ATG_water.sce

#D24 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 24, (first), Isomer=L
SwapRes 25, (second), Isomer=L
SwapRes 26, (third), Isomer=L
SwapRes 27, (fourth), Isomer=L
SwapRes 28, (fifth), Isomer=L
SwapRes 29, (six), Isomer=L
SwapRes 17, (cfirst), Isomer=L
SwapRes 16, (csecond), Isomer=L
SwapRes 15, (cthird), Isomer=L
SwapRes 14, (cfourth), Isomer=L
SwapRes 13, (cfifth), Isomer=L
SwapRes 12, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D24_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macro-target)_D24_ATG_water.sce

#D25 on G array
LoadSce (macro-target)_ATG.sce

SwapRes 25, (first), Isomer=L
SwapRes 26, (second), Isomer=L
SwapRes 27, (third), Isomer=L
SwapRes 28, (fourth), Isomer=L
SwapRes 29, (fifth), Isomer=L
SwapRes 30, (six), Isomer=L
SwapRes 16, (cfirst), Isomer=L
SwapRes 15, (csecond), Isomer=L
SwapRes 14, (cthird), Isomer=L
SwapRes 13, (cfourth), Isomer=L
SwapRes 12, (cfifth), Isomer=L
SwapRes 11, (csix), Isomer=L

ShowAll
SaveSce (macro-target)_D25_ATG.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D25_ATG_water.sce

#D26 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 26, (first), Isomer=L
SwapRes 27, (second), Isomer=L
SwapRes 28, (third), Isomer=L
SwapRes 29, (fourth), Isomer=L
SwapRes 30, (fifth), Isomer=L
SwapRes 31, (six), Isomer=L
SwapRes 15, (cfirst), Isomer=L
SwapRes 14, (csecond), Isomer=L
SwapRes 13, (cthird), Isomer=L
SwapRes 12, (cfourth), Isomer=L
SwapRes 11, (cfifth), Isomer=L
SwapRes 10, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D26_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D25_ATG_water.sce

#D27 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 27, (first), Isomer=L
SwapRes 28, (second), Isomer=L
SwapRes 29, (third), Isomer=L
SwapRes 30, (fourth), Isomer=L
SwapRes 31, (fifth), Isomer=L
SwapRes 32, (six), Isomer=L
SwapRes 14, (cfirst), Isomer=L
SwapRes 13, (csecond), Isomer=L
SwapRes 12, (cthird), Isomer=L
SwapRes 11, (cfourth), Isomer=L
SwapRes 10, (cfifth), Isomer=L
SwapRes 9, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D27_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D27_ATG_water.sce

#D28 on G array
LoadSce (macrotarget)_ATG.sce
SwapRes 28, (first), Isomer=L
SwapRes 29, (second), Isomer=L
SwapRes 30, (third), Isomer=L
SwapRes 31, (fourth), Isomer=L
SwapRes 32, (fifth), Isomer=L
SwapRes 33, (six), Isomer=L

SwapRes 13, (cfirst), Isomer=L
SwapRes 12, (csecond), Isomer=L
SwapRes 11, (cthird), Isomer=L
SwapRes 10, (cfourth), Isomer=L
SwapRes 9, (cfifth), Isomer=L
SwapRes 8, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D28_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D28_ATG_water.sce

#D29 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 29, (first), Isomer=L
SwapRes 30, (second), Isomer=L
SwapRes 31, (third), Isomer=L
SwapRes 32, (fourth), Isomer=L
SwapRes 33, (fifth), Isomer=L
SwapRes 34, (six), Isomer=L

SwapRes 12, (cfirst), Isomer=L
SwapRes 11, (csecond), Isomer=L
SwapRes 10, (cthird), Isomer=L
SwapRes 9, (cfourth), Isomer=L
SwapRes 8, (cfifth), Isomer=L
SwapRes 7, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D29_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D29_ATG_water.sce

#D30 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 30, (first), Isomer=L
SwapRes 31, (second), Isomer=L
SwapRes 32, (third), Isomer=L
SwapRes 33, (fourth), Isomer=L
SwapRes 34, (fifth), Isomer=L
SwapRes 35, (six), Isomer=L
SwapRes 11, (cfirst), Isomer=L
SwapRes 10, (csecond), Isomer=L
SwapRes 9, (cthird), Isomer=L
SwapRes 8, (cfourth), Isomer=L
SwapRes 7, (cfifth), Isomer=L
SwapRes 6, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D30_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D30_ATG_water.sce

#D31 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 31, (first), Isomer=L
SwapRes 32, (second), Isomer=L
SwapRes 33, (third), Isomer=L
SwapRes 34, (fourth), Isomer=L
SwapRes 35, (fifth), Isomer=L
SwapRes 36, (six), Isomer=L
SwapRes 10, (cfirst), Isomer=L
SwapRes 9, (csecond), Isomer=L
SwapRes 8, (cthird), Isomer=L
SwapRes 7, (cfourth), Isomer=L
SwapRes 6, (cfifth), Isomer=L
SwapRes 5, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D31_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D31_ATG_water.sce

#D32 on G array
LoadSce (macrotarget)_ATG.sce

SwapRes 32, (first), Isomer=L
SwapRes 33, (second), Isomer=L
SwapRes 34, (third), Isomer=L
SwapRes 35, (fourth), Isomer=L
SwapRes 36, (fifth), Isomer=L
SwapRes 37, (six), Isomer=L
SwapRes 9, (cfirst), Isomer=L
SwapRes 8, (csecond), Isomer=L
SwapRes 7, (cthird), Isomer=L
SwapRes 6, (cfourth), Isomer=L
SwapRes 5, (cfifth), Isomer=L
SwapRes 4, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D32_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D32_ATG_water.sce

=D33 on G array
LoadSce (macrotarget)_ATG.sce
SwapRes 33, (first), Isomer=L
SwapRes 34, (second), Isomer=L
SwapRes 35, (third), Isomer=L
SwapRes 36, (fourth), Isomer=L
SwapRes 37, (fifth), Isomer=L
SwapRes 38, (six), Isomer=L
SwapRes 8, (cfirst), Isomer=L
SwapRes 7, (csecond), Isomer=L
SwapRes 6, (cthird), Isomer=L
SwapRes 5, (cfourth), Isomer=L
SwapRes 4, (cfifth), Isomer=L
SwapRes 3, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D33_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D33_ATG_water.sce

=D34 on G array
LoadSce (macrotarget)_ATG.sce
SwapRes 34, (first), Isomer=L
SwapRes 35, (second), Isomer=L
SwapRes 36, (third), Isomer=L
SwapRes 37, (fourth), Isomer=L
SwapRes 38, (fifth), Isomer=L
SwapRes 39, (six), Isomer=L
SwapRes 7, (cfirst), Isomer=L
SwapRes 6, (csecond), Isomer=L
SwapRes 5, (cthird), Isomer=L
SwapRes 4, (cfourth), Isomer=L
SwapRes 3, (cfifth), Isomer=L
SwapRes 2, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D34_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D34_ATG_water.sce

#D35 on G array
LoadSce (macrotarget)_ATG.sce
SwapRes 35, (first), Isomer=L
SwapRes 36, (second), Isomer=L
SwapRes 37, (third), Isomer=L
SwapRes 38, (fourth), Isomer=L
SwapRes 39, (fifth), Isomer=L
SwapRes 40, (six), Isomer=L
SwapRes 6, (cfirst), Isomer=L
SwapRes 5, (csecond), Isomer=L
SwapRes 4, (cthird), Isomer=L
SwapRes 3, (cfourth), Isomer=L
SwapRes 2, (cfifth), Isomer=L
SwapRes 1, (csix), Isomer=L
ShowAll
SaveSce (macrotarget)_D35_ATG.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D35_ATG_water.sce

#C1 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 1, (first), Isomer=L
SwapRes 2, (second), Isomer=L
SwapRes 3, (third), Isomer=L
SwapRes 4, (fourth), Isomer=L
SwapRes 5, (fifth), Isomer=L
SwapRes 6, (six), Isomer=L
SwapRes 35, (csix), Isomer=L
SwapRes 36, (cfifth), Isomer=L
SwapRes 37, (cfourth), Isomer=L
SwapRes 38, (cthird), Isomer=L
SwapRes 39, (csecond), Isomer=L
SwapRes 40, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C1_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C1_ATGC_water.sce

#C2 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 2, (first), Isomer=L
SwapRes 3, (second), Isomer=L
SwapRes 4, (third), Isomer=L
SwapRes 5, (fourth), Isomer=L
SwapRes 6, (fifth), Isomer=L
SwapRes 7, (six), Isomer=L
SwapRes 34, (csix), Isomer=L
SwapRes 35, (cfifth), Isomer=L
SwapRes 36, (cfourth), Isomer=L
SwapRes 37, (cthird), Isomer=L
SwapRes 38, (csecond), Isomer=L
SwapRes 39, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C2_ATGC.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C2_ATGC_water.sce

#C3 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 3, (first), Isomer=L
SwapRes 4, (second), Isomer=L
SwapRes 5, (third), Isomer=L
SwapRes 6, (fourth), Isomer=L
SwapRes 7, (fifth), Isomer=L
SwapRes 8, (six), Isomer=L
SwapRes 33, (csix), Isomer=L
SwapRes 34, (cfifth), Isomer=L
SwapRes 35, (cfourth), Isomer=L
SwapRes 36, (cthird), Isomer=L
SwapRes 37, (csecond), Isomer=L
SwapRes 38, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C3_ATGC.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C3_ATGC_water.sce

#C4 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 4, (first), Isomer=L
SwapRes 5, (second), Isomer=L
SwapRes 6, (third), Isomer=L
SwapRes 7, (fourth), Isomer=L
SwapRes 8, (fifth), Isomer=L
SwapRes 9, (six), Isomer=L
SwapRes 32, (csix), Isomer=L
SwapRes 33, (cfifth), Isomer=L
SwapRes 34, (cfourth), Isomer=L
SwapRes 35, (cthird), Isomer=L
SwapRes 36, (csecond), Isomer=L
SwapRes 37, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C4_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C4_ATGC_water.sce

#C5 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 5, (first), Isomer=L
SwapRes 6, (second), Isomer=L
SwapRes 7, (third), Isomer=L
SwapRes 8, (fourth), Isomer=L
SwapRes 9, (fifth), Isomer=L
SwapRes 10, (six), Isomer=L
SwapRes 31, (csix), Isomer=L
SwapRes 32, (cfifth), Isomer=L
SwapRes 33, (cfourth), Isomer=L
SwapRes 34, (cthird), Isomer=L
SwapRes 35, (csecond), Isomer=L
SwapRes 36, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C5_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C5_ATGC_water.sce

#C6 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 6, (first), Isomer=L
SwapRes 7, (second), Isomer=L
SwapRes 8, (third), Isomer=L
SwapRes 9, (fourth), Isomer=L
SwapRes 10, (fifth), Isomer=L
SwapRes 11, (six), Isomer=L
SwapRes 30, (csix), Isomer=L
SwapRes 31, (cfifth), Isomer=L
SwapRes 32, (cfourth), Isomer=L
SwapRes 33, (cthird), Isomer=L
SwapRes 34, (csecond), Isomer=L
SwapRes 35, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C6_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C6_ATGC_water.sce

#C7 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 7, (first), Isomer=L
SwapRes 8, (second), Isomer=L
SwapRes 9, (third), Isomer=L
SwapRes 10, (fourth), Isomer=L
SwapRes 11, (fifth), Isomer=L
SwapRes 12, (six), Isomer=L
SwapRes 29, (csix), Isomer=L
SwapRes 30, (cfifth), Isomer=L
SwapRes 31, (cfourth), Isomer=L
SwapRes 32, (cthird), Isomer=L
SwapRes 33, (csecond), Isomer=L
SwapRes 34, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C7_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C7_ATGC_water.sce

#C8 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 8, (first), Isomer=L
SwapRes 9, (second), Isomer=L
SwapRes 10, (third), Isomer=L
SwapRes 11, (fourth), Isomer=L
SwapRes 12, (fifth), Isomer=L
SwapRes 13, (six), Isomer=L
SwapRes 28, (csix), Isomer=L
SwapRes 29, (cfifth), Isomer=L
SwapRes 30, (cfourth), Isomer=L
SwapRes 31, (cthird), Isomer=L
SwapRes 32, (csecond), Isomer=L
SwapRes 33, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C8_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macroTarget) _C9_ATGC_water.sce

#C9 on C array
LoadSce (macroTarget) _ATGC.sce

SwapRes 9, (first), Isomer=L
SwapRes 10, (second), Isomer=L
SwapRes 11, (third), Isomer=L
SwapRes 12, (fourth), Isomer=L
SwapRes 13, (fifth), Isomer=L
SwapRes 14, (six), Isomer=L

SwapRes 27, (csix), Isomer=L
SwapRes 28, (cfifth), Isomer=L
SwapRes 29, (cfourth), Isomer=L
SwapRes 30, (cthird), Isomer=L
SwapRes 31, (csecond), Isomer=L
SwapRes 32, (cfirst), Isomer=L

ShowAll
SaveSce (macroTarget) _C9_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macroTarget) _C9_ATGC_water.sce

#C10 on C array
LoadSce (macroTarget) _ATGC.sce

SwapRes 10, (first), Isomer=L
SwapRes 11, (second), Isomer=L
SwapRes 12, (third), Isomer=L
SwapRes 13, (fourth), Isomer=L
SwapRes 14, (fifth), Isomer=L
SwapRes 15, (six), Isomer=L

SwapRes 26, (csix), Isomer=L
SwapRes 27, (cfifth), Isomer=L
SwapRes 28, (cfourth), Isomer=L
SwapRes 29, (cthird), Isomer=L
SwapRes 30, (csecond), Isomer=L
SwapRes 31, (cfirst), Isomer=L

ShowAll
SaveSce (macroTarget) _C10_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macroTarget) _C10_ATGC_water.sce

#C11 on C array
LoadSce (macroTarget) _ATGC.sce
SwapRes 11, (first), Isomer=L
SwapRes 12, (second), Isomer=L
SwapRes 13, (third), Isomer=L
SwapRes 14, (fourth), Isomer=L
SwapRes 15, (fifth), Isomer=L
SwapRes 16, (six), Isomer=L
SwapRes 25, (csix), Isomer=L
SwapRes 26, (cfifth), Isomer=L
SwapRes 27, (cfourth), Isomer=L
SwapRes 28, (cthird), Isomer=L
SwapRes 29, (csecond), Isomer=L
SwapRes 30, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C11_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C11_ATGC_water.sce

#C12 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 12, (first), Isomer=L
SwapRes 13, (second), Isomer=L
SwapRes 14, (third), Isomer=L
SwapRes 15, (fourth), Isomer=L
SwapRes 16, (fifth), Isomer=L
SwapRes 17, (six), Isomer=L
SwapRes 24, (csix), Isomer=L
SwapRes 25, (cfifth), Isomer=L
SwapRes 26, (cfourth), Isomer=L
SwapRes 27, (cthird), Isomer=L
SwapRes 28, (csecond), Isomer=L
SwapRes 29, (cfirst), Isomer=L
ShowAll
SaveSce (macrotarget)_C12_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C12_ATGC_water.sce

#C13 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 13, (first), Isomer=L
SwapRes 14, (second), Isomer=L
SwapRes 15, (third), Isomer=L
SwapRes 16, (fourth), Isomer=L
SwapRes 17, (fifth), Isomer=L
SwapRes 18, (six), Isomer=L
SwapRes 23, (csix), Isomer=L
SwapRes 24, (cfifth), Isomer=L
SwapRes 25, (cfourth), Isomer=L
SwapRes 26, (cthird), Isomer=L
SwapRes 27, (csecond), Isomer=L
SwapRes 28, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C13_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C13_ATGC_water.sce

#C14 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 14, (first), Isomer=L
SwapRes 15, (second), Isomer=L
SwapRes 16, (third), Isomer=L
SwapRes 17, (fourth), Isomer=L
SwapRes 18, (fifth), Isomer=L
SwapRes 19, (six), Isomer=L
SwapRes 22, (csix), Isomer=L
SwapRes 23, (cfifth), Isomer=L
SwapRes 24, (cfourth), Isomer=L
SwapRes 25, (cthird), Isomer=L
SwapRes 26, (csecond), Isomer=L
SwapRes 27, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C14_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C14_ATGC_water.sce

#C15 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 15, (first), Isomer=L
SwapRes 16, (second), Isomer=L
SwapRes 17, (third), Isomer=L
SwapRes 18, (fourth), Isomer=L
SwapRes 19, (fifth), Isomer=L
SwapRes 20, (six), Isomer=L
SwapRes 21, (csix), Isomer=L
SwapRes 22, (cfifth), Isomer=L
SwapRes 23, (cfourth), Isomer=L
SwapRes 24, (cthird), Isomer=L

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SwapRes 25, (csecond), Isomer=L
SwapRes 26, (cfirst), Isomer=L

ShowAll
SaveSce (macrotarget)_C15_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_C15_ATGC_water.sce

#D21 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 21, (first), Isomer=L
SwapRes 22, (second), Isomer=L
SwapRes 23, (third), Isomer=L
SwapRes 24, (fourth), Isomer=L
SwapRes 25, (fifth), Isomer=L
SwapRes 26, (six), Isomer=L
SwapRes 20, (cfirst), Isomer=L
SwapRes 19, (csecond), Isomer=L
SwapRes 18, (cthird), Isomer=L
SwapRes 17, (cfourth), Isomer=L
SwapRes 16, (cfifth), Isomer=L
SwapRes 15, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D21_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D21_ATGC_water.sce

#D22 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 22, (first), Isomer=L
SwapRes 23, (second), Isomer=L
SwapRes 24, (third), Isomer=L
SwapRes 25, (fourth), Isomer=L
SwapRes 26, (fifth), Isomer=L
SwapRes 27, (six), Isomer=L
SwapRes 19, (cfirst), Isomer=L
SwapRes 18, (csecond), Isomer=L
SwapRes 17, (cthird), Isomer=L
SwapRes 16, (cfourth), Isomer=L
SwapRes 15, (cfifth), Isomer=L
SwapRes 14, (csix), Isomer=L

ShowAll
SaveSce (macrotarget) _D22_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget) _D22_ATGC_water.sce

#D23 on C array
LoadSce (macrotarget) _ATGC.sce

SwapRes 23, (first), Isomer=L
SwapRes 24, (second), Isomer=L
SwapRes 25, (third), Isomer=L
SwapRes 26, (fourth), Isomer=L
SwapRes 27, (fifth), Isomer=L
SwapRes 28, (six), Isomer=L
SwapRes 18, (cfirst), Isomer=L
SwapRes 17, (csecond), Isomer=L
SwapRes 16, (cthird), Isomer=L
SwapRes 15, (cfourth), Isomer=L
SwapRes 14, (cfifth), Isomer=L
SwapRes 13, (csix), Isomer=L

ShowAll
SaveSce (macrotarget) _D23_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget) _D23_ATGC_water.sce

#D24 on C array
LoadSce (macrotarget) _ATGC.sce

SwapRes 24, (first), Isomer=L
SwapRes 25, (second), Isomer=L
SwapRes 26, (third), Isomer=L
SwapRes 27, (fourth), Isomer=L
SwapRes 28, (fifth), Isomer=L
SwapRes 29, (six), Isomer=L
SwapRes 17, (cfirst), Isomer=L
SwapRes 16, (csecond), Isomer=L
SwapRes 15, (cthird), Isomer=L
SwapRes 14, (cfourth), Isomer=L
SwapRes 13, (cfifth), Isomer=L
SwapRes 12, (csix), Isomer=L

ShowAll
SaveSce (macrotarget) _D24_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget) _D24_ATGC_water.sce
#D25 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 25, (first), Isomer=L
SwapRes 26, (second), Isomer=L
SwapRes 27, (third), Isomer=L
SwapRes 28, (fourth), Isomer=L
SwapRes 29, (fifth), Isomer=L
SwapRes 30, (six), Isomer=L

SwapRes 16, (cfirst), Isomer=L
SwapRes 15, (csecond), Isomer=L
SwapRes 14, (cthird), Isomer=L
SwapRes 13, (cfourth), Isomer=L
SwapRes 12, (cfifth), Isomer=L
SwapRes 11, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D25_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D25_ATGC_water.sce

#D26 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 26, (first), Isomer=L
SwapRes 27, (second), Isomer=L
SwapRes 28, (third), Isomer=L
SwapRes 29, (fourth), Isomer=L
SwapRes 30, (fifth), Isomer=L
SwapRes 31, (six), Isomer=L

SwapRes 15, (cfirst), Isomer=L
SwapRes 14, (csecond), Isomer=L
SwapRes 13, (cthird), Isomer=L
SwapRes 12, (cfourth), Isomer=L
SwapRes 11, (cfifth), Isomer=L
SwapRes 10, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D26_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D26_ATGC_water.sce

#D27 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 27, (first), Isomer=L
SwapRes 28, (second), Isomer=L
SwapRes 29, (third), Isomer=L
SwapRes 30, (fourth), Isomer=L
SwapRes 31, (fifth), Isomer=L
SwapRes 32, (six), Isomer=L

SwapRes 14, (cfirst), Isomer=L
SwapRes 13, (csecond), Isomer=L
SwapRes 12, (cthird), Isomer=L
SwapRes 11, (cfourth), Isomer=L
SwapRes 10, (cfifth), Isomer=L
SwapRes 9, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D27_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D27_ATGC_water.sce

#D28 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 28, (first), Isomer=L
SwapRes 29, (second), Isomer=L
SwapRes 30, (third), Isomer=L
SwapRes 31, (fourth), Isomer=L
SwapRes 32, (fifth), Isomer=L
SwapRes 33, (six), Isomer=L

SwapRes 13, (cfirst), Isomer=L
SwapRes 12, (csecond), Isomer=L
SwapRes 11, (cthird), Isomer=L
SwapRes 10, (cfourth), Isomer=L
SwapRes 9, (cfifth), Isomer=L
SwapRes 8, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D28_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D28_ATGC_water.sce

#D29 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 29, (first), Isomer=L
SwapRes 30, (second), Isomer=L
SwapRes 31, (third), Isomer=L
SwapRes 32, (fourth), Isomer=L
SwapRes 33, (fifth), Isomer=L
SwapRes 34, (six), Isomer=L

SwapRes 12, (cfirst), Isomer=L
SwapRes 11, (csecond), Isomer=L
SwapRes 10, (cthird), Isomer=L
SwapRes 9, (cfourth), Isomer=L
SwapRes 8, (cfifth), Isomer=L
SwapRes 7, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D29_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D29_ATGC_water.sce

#D30 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 30, (first), Isomer=L
SwapRes 31, (second), Isomer=L
SwapRes 32, (third), Isomer=L
SwapRes 33, (fourth), Isomer=L
SwapRes 34, (fifth), Isomer=L
SwapRes 35, (six), Isomer=L

SwapRes 11, (cfirst), Isomer=L
SwapRes 10, (csecond), Isomer=L
SwapRes 9, (cthird), Isomer=L
SwapRes 8, (cfourth), Isomer=L
SwapRes 7, (cfifth), Isomer=L
SwapRes 6, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D30_ATGC.sce
CleanAll
FillCellWater Density=0.997, Probe=1.4, BumpSum=1.0, DisMax=0
SwitchObj 3, off
SaveSce (macrotarget)_D30_ATGC_water.sce

#D31 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 31, (first), Isomer=L
SwapRes 32, (second), Isomer=L
SwapRes 33, (third), Isomer=L
SwapRes 34, (fourth), Isomer=L
SwapRes 35, (fifth), Isomer=L
SwapRes 36, (six), Isomer=L

SwapRes 10, (cfirst), Isomer=L
SwapRes 9, (csecond), Isomer=L
SwapRes 8, (cthird), Isomer=L
SwapRes 7, (cfourth), Isomer=L
SwapRes 6, (cfifth), Isomer=L
SwapRes 5, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D31_ATGC.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D31_ATGC_water.sce

#D32 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 32, (first), Isomer=L
SwapRes 33, (second), Isomer=L
SwapRes 34, (third), Isomer=L
SwapRes 35, (fourth), Isomer=L
SwapRes 36, (fifth), Isomer=L
SwapRes 37, (six), Isomer=L

SwapRes 9, (cfirst), Isomer=L
SwapRes 8, (csecond), Isomer=L
SwapRes 7, (cthird), Isomer=L
SwapRes 6, (cfourth), Isomer=L
SwapRes 5, (cfifth), Isomer=L
SwapRes 4, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D32_ATGC.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D32_ATGC_water.sce

#D33 on C array
LoadSce (macrotarget)_ATGC.sce

SwapRes 33, (first), Isomer=L
SwapRes 34, (second), Isomer=L
SwapRes 35, (third), Isomer=L
SwapRes 36, (fourth), Isomer=L
SwapRes 37, (fifth), Isomer=L
SwapRes 38, (six), Isomer=L

SwapRes 8, (cfirst), Isomer=L
SwapRes 7, (csecond), Isomer=L
SwapRes 6, (cthird), Isomer=L
SwapRes 5, (cfourth), Isomer=L
SwapRes 4, (cfifth), Isomer=L
SwapRes 3, (csix), Isomer=L

ShowAll
SaveSce (macrotarget)_D33_ATGC.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D33_ATGC_water.sce
#D34 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 34, (first), Isomer=L
SwapRes 35, (second), Isomer=L
SwapRes 36, (third), Isomer=L
SwapRes 37, (fourth), Isomer=L
SwapRes 38, (fifth), Isomer=L
SwapRes 39, (six), Isomer=L
SwapRes 7, (cfirst), Isomer=L
SwapRes 6, (csecond), Isomer=L
SwapRes 5, (cthird), Isomer=L
SwapRes 4, (cfourth), Isomer=L
SwapRes 3, (cfifth), Isomer=L
SwapRes 2, (csix), Isomer=L
ShowAll
SaveSce (macrotarget)_D34_ATGC.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D34_ATGC_water.sce

#D35 on C array
LoadSce (macrotarget)_ATGC.sce
SwapRes 35, (first), Isomer=L
SwapRes 36, (second), Isomer=L
SwapRes 37, (third), Isomer=L
SwapRes 38, (fourth), Isomer=L
SwapRes 39, (fifth), Isomer=L
SwapRes 40, (six), Isomer=L
SwapRes 6, (cfirst), Isomer=L
SwapRes 5, (csecond), Isomer=L
SwapRes 4, (cthird), Isomer=L
SwapRes 3, (cfourth), Isomer=L
SwapRes 2, (cfifth), Isomer=L
SwapRes 1, (csix), Isomer=L
ShowAll
SaveSce (macrotarget)_D35_ATGC.sce
CleanAll
FillCellWater Density=0.997,Probe=1.4,BumpSum=1.0,DisMax=0
SwitchObj 3,off
SaveSce (macrotarget)_D35_ATGC_water.sce
**md and analysis for scanning array Macro**

# Runs the simulations for one consensus site on all four backgrounds of the DNA. Must run for each of the sites allowing for faster generation of data but requiring more RAM to run. Much of the script is modifications and duplications made to the md_analysis macro and md_analyseres macros from YASARA.

# The structure to simulate must be present with a .pdb or .sce extension. If a .sce (=YASARA scene) file is present, the cell must have been added.

# You can either set the target structure by clicking on Options > Macro > Set target,
# or by uncommenting the line below and specifying it directly.
# MacroTarget = 'c:\MyProject\1crn'

# Extension of the cell on each side of the protein
# '10' means that the cell will be 20 Å larger than the protein
extension=10

# pH at which the simulation should be run, by default physiological pH
ph=7.4

# NaCl concentration in mass percent (0.9% is a physiological solution)
acl=0.9

# Simulation temperature
# If you run at a temperature that differs from 298K, you also need
# to adapt the pressure control below, look in the PressureCtrl documentation.
temperature='298K'

# Pressure control mode
# Default: Rescale the cell such that residues named HOH reach a density
# of 0.997 g/l.
# For solvents other than water, you have to create your own solvent box
# as described in the FillCellObj documentation and save it as
# .._solvent.sce.
density=0.997
pressurectrl='SolventProbe,Name=HOH,Density=(density)'

# Alternative: Uncomment below to calculate the pressure from the virial and
# rescale the cell to reach a pressure of 1 bar. Use this method if you do not
# know the correct density.
# pressurectrl='Manometer,Pressure=1'

# Constrain bond lengths to hydrogens and water bond angles to allow a larger timestep
# If set to 'yes', the MD will run faster, but will be a bit less accurate
# constrain='no'

# The format used to save the trajectories, sim or xtc
format='sim'
# Duration of the simulation, alternatively use e.g. 'duration=5200' to simulate for 5000 picoseconds
duration=520

# Flag to use a cubic simulation cell. This makes sure that also elongated molecules can rotate freely during very long simulations. If set to 0, the simulation cell will fit the solute more tightly, speeding up the simulation.
cubic=1

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Normally no change required below this point
# ==============================================================
RequireVersion 9.9.25

# Keep the solute from diffusing around and crossing periodic boundaries
CorrectDrift On

# Treat all simulation warnings as errors that stop the macro
WarnIsError On

# Do we have a target?
if MacroTarget==''
    RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to choose a target structure"

Clear
# Do we already have a scene with water or other solvent?
waterscene = FileSize (MacroTarget)_water.sce
solventscene = FileSize (MacroTarget)_solvent.sce
if waterscene
    LoadSce (MacroTarget)_water
elif solventscene
    LoadSce (MacroTarget)_solvent
else
    # No scene with solvent present yet
    # Do we have a scene at all?
    scene = FileSize (MacroTarget).sce
    if scene
        LoadSce (MacroTarget)
    else

# No scene present, assume it's a PDB or YOB file
for type in 'pdb','yob','Error'
    size = FileSize (MacroTarget).(type)
    if size
        obj = Load(type) (MacroTarget)
        # Align object with major axes to minimize cell size
        NiceOriObj (obj)
        break
    if type=='Error'
        RaiseError "Initial structure not found. Make sure to create a project directory and place the structure there"
# Prepare the structure for simulation
CleanAll
if Structure
    # Optimize the hydrogen-bonding network (more stable trajectories)
    OptHydAll
    # Create the simulation cell
    Cell Auto,Extension=(extension)
    if cubic
        # And make it cubic, taking the length of the X-axis, which is always the longest
        l = Cell
        Cell (l),(l),(l)
        SaveSce (MacroTarget)
    # Fill with water (always needs periodic boundaries), predict pKas, place counter ions
    Boundary periodic
    Experiment Neutralization
    WaterDensity (density)
    pH (ph)
    NaCl (nacl)
    pKaFile (MacroTarget).pka
    Speed Fast
    Experiment On
    Wait ExpEnd
    # Save scene with water
    SaveSce (MacroTarget)_water
# Choose timestep and activate constraints
if constrain=='yes'
    # Constrain bond lengths to hydrogens
    FixBond all,Element H
    # Constrain bond angles in water
    FixAngle Water,Water,Water
    # Multiple timestep: 1.3333 femtoseconds for intramolecular and 3*1.3333 = 4 fs for intermolecular forces
    TimeStep 3,1.3333
    ts=4
    # Save simulation snapshots every 6250 simulation steps
    # (with a timestep of 4 femtoseconds, that's 6540*4 fs = 25 picoseconds).
    savesteps=6250
else
    # Remove any constraints
FreeBond all,all
FreeAngle all,all,all
# Smaller timestep, since we don't use constraints: 2*1.25 = 2.5 fs
TimeStep 2,1.25
ts=2.5
# Save simulation snapshots every 10000 simulation steps
# (with a timestep of 2.5 femtoseconds, that's 10000*2.5 fs = 25 picoseconds).
savesteps=10000

# Temperature
Temp (temperature)
# Make sure all atoms are free to move
FreeAll
# Already a snapshot/trajectory present?
i=00000
filename='(MacroTarget)(i).(format)'
running = FileSize (filename)
if not running
    # Perform energy minimization
    Experiment Minimization
    Experiment On
    Wait ExpEnd
    # And now start the real simulation
    Sim On
else
    # Simulation has been running before
    ShowMessage "Simulation has been running before, loading last snapshot..."
    Wait 1
    # Switch console off to load the snapshots quickly
    Console Off
    if format=='sim'
        # Find and load the last 'sim' snapshot
        do
            i = i+1
            found = FileSize (MacroTarget)(i).sim
            while found
                i=i-1
                LoadSim (MacroTarget)(i)
            else
                # XTC format requires that the entire trajectory is read in to find the last one
                do
                    i = i+1
                    eof,time = LoadXTC (filename),(i)
                    ShowMessage 'Searching XTC trajectory for last snapshot, showing snapshot (i) at (0+time) fs'
                    Sim Pause
                    Wait 1
                    while !eof
                        Sim Continue
                # Adjust savesteps to save snapshots in the same interval as previously
                if i>0
t = Time
    savesteps=0+t/(ts*i)
    #print 'Time=(t), TimeStep=(ts), savesteps=(savesteps)'
HideMessage

# Set temperature and pressure control
TempCtrl Rescale
PressureCtrl (pressurectrl)

# Uncomment to add distance constraints
# AddSpring O Res Lys 80, H Res Glu 84, Len=1.9

# And finally, make sure that future snapshots are saved
Save(format) (filename),(savesteps)

if duration=='forever'
    Console On
    Wait forever
else
    Console Off
    # Wait for given number of picoseconds
    do
        Wait 10
        t = Time
    while t<duration*1000
    Sim Off

# Number of the object whose RMSDs from the starting conformation will be calculated
# If the protein is an oligomer, check the documentation of the 'Sup' command at 'analyzing a simulation' to avoid pitfalls.
currobj = 1

# Forcefield to use (these are all YASARA commands, so no '=' used)
# Use YASARA2 in YASARA Structure to include a quality Z-score
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# The B-factors calculated from the root-mean-square fluctuations can be too large to fit them
# into the PDB file's B-factor column. Replace e.g. 1.0 with 0.1 to scale them down to 10%
bfactorscale=1.0

# Flag to save a PDB file of the solute snapshots for further analysis
pidebar=0

# Selection of atoms to include for 'Calpha' RMSD calculation (also consider DNA/RNA)
casel='CA Protein or Cl* NucAcid'

# Selection of atoms for which the dynamic cross-correlation matrix (DCCM) should be visualized.
# Here are some typical examples:
# dccmsel='' - Don't calculate the DCCM, the default
# dccmsel='Atom CA Protein' - Calculate the DCCM for protein Calpha atoms
# dccmsel='Res Protein' - Calculate the DCCM for protein residue centers
dccmsel=''

# Selection of atoms for which the radial distribution function (RDF) should be visualized
# Here are some examples:
# rdfsel='' - Don't calculate the RDF, the default
# rdfsel='O Res HOH,O Res HOH,Bins=40,BinWidth=0.25'
# - Calculate the RDF of water in 40 bins, each 0.25 A wide (thus up to 10 A).
# rdfsel='CG Res Asp 120,ND1 Res His 200,Bins=20,BinWidth=0.5'
# - Calculate the RDF between two specific atoms in 20 bins, each 0.25 A wide
# (thus again up to 10 A). Note that you may have to save more snapshots than
# usually in md_run.mcr to avoid problems with sparse data and noisy RDF results.
rdfsel=''

# First snapshot to be analyzed, increase number to ignore an equilibration period.
# (By default, md_run.mcr saves snapshots every 25ps, choosing 40 thus starts the analysis after 1 nanosecond)
firstsnapshot=0

# No change required below this point
# --------------------------------------

# Do we have a target?
if MacroTarget=''
   RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to choose a target structure"

Clear
Console Off
# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
   RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water
calphas = CountAtom (casel)
if calphas>0 and calphas<3
    # We cannot superpose 1 or 2 Calpha atoms
casel='None'
ShowMessage "Preparing analysis, please wait..."
Wait 1

# See if structure validation checks should be done (require YASARA2 force
field)
checked=0
fof = ForceField
if fof=='YASARA2'
    checked=1

# Duplicate the intial object for RMSD calculation
startobj = DuplicateObj (currobj)
RemoveObj (startobj)

i=00000+firstsnapshot
emin=1e99
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    # Add time in picoseconds to table
    simtime = Time
    ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
    Wait 1
    Tabulate (simtime/1000)
    # Get energy components, including packing energies for YASARA2 force
field
    if checked
        ebndlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i),pa
cking1,packing3 = EnergyAll All
    else
        ebndlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i) =
        EnergyAll All
        packing1=0
        packing3=0
       elist(i) =
        ebndlist(i)+eanglist(i)+edihlist(i)+eplnlist(i)+ecoulist(i)+evdwlist(i)+pa
cking1+packing3
    # The following examples provide a few hints for other things to
analyze.
    # If you uncomment one of the examples, keep in mind that every value
you
## tabulate becomes an additional column in the table, so you must increase the
## 'Columns' parameter of the SaveTab command further below (and the table
## header will also no longer indicate the proper results unless you adapt it).

### Example: Measure the distance between the carboxyl group of Glu 123 (Cdelta)
and the guanidinium group of Arg 345 (Czeta):
```
Tabulate Distance CD Res Glu 123, CZ Res Arg 345
```

### Example: Measure the distance between two centers of mass, e.g. the loop from
residue Ala 205 to Glu 210, and the ligand NAD:
```
cenA() = GroupCenter Res Ala 205 - Glu 210, Type=Mass
cenB() = GroupCenter Res NAD, Type=Mass
Tabulate (norm (cenA-cenB))
```

### Example: Check if the carboxyl group of Glu 123 and the guanidinium group of
Arg 345 are currently hydrogen-bonded (1) or not (0):
```
hbolist() = ListHBoAtom Sidechain Res Glu 123, Sidechain Res Arg 345
Tabulate (count hbolist>0)
```

### Example: Count the number of atoms in molecule A that are hydrogen bonded to B
```
hbolist() = ListHBoAtom Mol A,Mol B
Tabulate (count hbolist)
```

### Example: Calculate the current potential energy of residue Glu 123:
```
Tabulate EnergyRes Glu 123
```

### Example: Calculate the backbone RMSD for residues 1-120:
```
Tabulate SupAtom Backbone Res 1-120 Obj (currobj),Backbone Res 1-120 Obj (startobj)
```

### Save the minimum energy structure (ignoring solvent-solvent interactions)
```
e = EnergyObj (currobj)
if checked
    # Calculate structure validation Z-scores, using the formula from homology modeling
    for type in 'dihedrals','packing1d','packing3d'
        zscore(type) = CheckObj (currobj),(type)
    zscorelist(i)=zscoredihedrals*0.145+zscorepacking1d*0.390+zscorepacking3d*0.465
if rdfsel=''
    # Collect data for radial distribution function
    BinDistance (rdfsel)
Sim Off
if e<emin
    emin=e
```
SaveSce (MacroTarget)_energymin
if pdbsaved
# Save a PDB file of the solute
SavePDB (currobj),(MacroTarget)_(i)
# Add CA, backbone and heavy atom RMSDs to table
AddObj (startobj)
# Trick: If the solute object contains neither CA nor backbone atoms,
# we simply assign the SupAtom error code (=0)
carmsdlist(i) = SupAtom (casel) and Obj (currobj), (casel) and Obj (startobj)
bbbrmsdlist(i) = SupAtom Backbone Obj (currobj), Backbone Obj (startobj)
aarmsdlist(i) = SupAtom Element !H Obj (currobj), Element !H Obj
AddObj (startobj)
# Add results to table
Tabulate (elist(i)),(ebndlist(i)),(eanglist(i)),(edihlist(i)),(eplnlist(i)),
(ecoulislist(i)),(evdwlist(i)),
(carmsdlist(i)),(bbbrmsdlist(i)),(aarmsdlist(i))
if checked
   Tabulate (zscorelist(i))
# Add the current atom positions to internal table to obtain RMSF and average positions
AddPosAtom Obj (currobj)
RemoveObj (startobj)
# Next snapshot
i=i+1
if !i
   RaiseError "This macro is meant to analyze a molecular dynamics trajectory created with md_run, but none was found in this directory"

   # Add average results to table
   Tabulate 'Average', (mean elist), (mean ebndlist), (mean eanglist), (mean edihlist),
   (mean eplnlist),
   (mean ecoulislist), (mean evdwlist), (mean carmsdlist), (mean
   bbrmsdlist), (mean aarmsdlist)
   header='____Time[ps] Energy[(EnergyUnit)]____Bond _______Angle
   ______Dihedral ___Planarity _____Coulomb _________VdW _RMSDs[A]:CA __
   Backbone ___HeavyAtoms'
   if checked
      header=header+' QualityScore'
   Tabulate (mean zscorelist)
# Save main analysis table
SaveTab
default,(MacroTarget)_analysis,Format=Text,Columns=(11+checked),NumFormat=12.3f,(header)

# Calculate time-average structure and set B-factors according to RMSF
AveragePosAtom Obj (currobj)
RMSFAtom Obj (currobj), Unit=BFactor
if bfactorscale!=1.0
   # Scale B-factors so that they fit into the PDB format
   first,last=SpanAtom Obj (currobj)
   for i=first to last
bf=BFactorAtom (i)
BFactorAtom (i),(bf*bftorscale)
# The time average structure has incorrect covalent geometry and should be energy minimized
SavePDB (currobj),(MacroTarget)_average

# Example: Create an additional RMSF file, in case B-factors are too large for the PDB format
DelTab default
first,last = SpanAtom Obj (currobj)
rmsflist() = RMSFAtom Obj (currobj)
for i=first to last
    res = ListAtom (i),Format='RESNAME,RESNUM'
    Tabulate (i),(res),(rmsflist(i-first+1))
SaveTab
default,(MacroTarget)_rmsf,Format=Text,Columns=4,NumFormat=8.2f,"RMSF Table"

if rdfsel!=''
    # Additionally calculate and show the radial distribution function (RDF).
    MakeTab RDF,Dimensions=1
    Tabulate RDF
    SaveTab RDF,(MacroTarget)_rdf,Format=Text,Columns=1,NumFormat=6.3f,
    'Radial distribution function with parameters (rdfsel)'
    obj = ShowTab RDF,Width=1.0,Range=10,MinCol=Blue,MaxCol=Yellow
    PosObj (obj),X=0,Y=-12,Z=31
    RotateObj (obj),X=-90
    SaveSce (MacroTarget)_rdf
    DelObj (obj)

if dccmsel!=''
    # Additionally calculate and show the dynamic cross-correlation matrix (DCCM).
    # This matrix correlates the displacements from the time average structure,
    # see the documentation of the 'DCCM' command for details.
    # First get the number of selected units, i.e. the rows/columns in the matrix
    units = Count(dccmsel)
    if !units
        RaiseError 'The DCCM selection (dccmsel) did not match any atoms'
    # Take the time average structure as the start object to superpose onto
    DelObj (startobj)
    startobj = DuplicateObj (currobj)
    RemoveObj (startobj)
    # Loop over the snapshots a second time to calculate the displacements from the time average
    i=00000+firstsnapshot
    while 1
        # See if next snapshot is present
        sim = FileSize (MacroTarget)(i).sim
if not sim
    break
# Yes, load it
LoadSim (MacroTarget)(i)
Sim Pause
ShowMessage 'Calculating dynamic cross-correlation matrix, analyzing
snapshot (0+i)...
Wait 1
Sim Off
# Superpose snapshot on the time average structure
AddObj (startobj)
SupAtom (casel) and Obj (currobj),(casel) and Obj (startobj)
# Add the current displacements to an internal table to obtain the
DCCM
AddDisp(dccmsel) Obj (currobj),(dccmsel) Obj (startobj)
RemoveObj (startobj)
# Next snapshot
i=i+1
# Store the DCCM in a table
MakeTab DCCM,Dimensions=2,Columns=(units)
Tabulate DCCM
# Visualize the DCCM
pointwidth=1.
height=5.
dccmobj1 = ShowTab DCCM,Width=(pointwidth),Range=(height),Min=-1,Max=1.0
# By default, ShowTab shows the minimum at Z=0, move so that correlation
0 is at Z=0
MoveObj (dccmobj1),Z=(height*0.5)
# Visualize the zero level with a flat DCCM wireframe
dccmobj2 = ShowTab DCCM,Width=(pointwidth),Range=0,Min=-1,Max=1.0
dccmobj3 = ShowWireObj (dccmobj2),Static,Mesh=Solid
DelObj (dccmobj2)
PointPar Radius=0.5,Plastic=No
NameObj (dccmobj3),ZeroLevel
RotateObj (dccmobj1) (dccmobj3),X=180
# Create a text object with the residue names and the table header
textwidth=pointwidth*units*2
textobj1 = MakeTextObj Units,Width=(textwidth),Height=(textwidth)
Font Arial,Height=(pointwidth*0.6),Color=Yellow,Depth=0.5,DepthCol=Red
idlist() = List(dccmsel) Obj (currobj),Format='MOLNAME RESName RESNUM'
for i=1 to units
    PosText X=(textwidth*0.5+pointwidth*-0.5*(units+6)),
    Y=(textwidth*0.5+pointwidth*(0.5*units-i)),justify=left
    Print (idlist(i))
# Duplicate the labels at the bottom
textobj2 = DuplicateObj (textobj1)
RotateObj (textobj2),Z=90
DelObj not (dccmobj1) (dccmobj3) (join textobj)
RenumberObj all
# Save the matrix
SaveTab
DCCM,(MacroTarget)_dccm,Format=Text,Columns=(units),NumFormat=6.3f,
    'Dynamic Cross-Correlation Matrix for (units) selected units'
# Save the visualized matrix
SaveSce (MacroTarget)_dccm
HideMessage

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Consider protein residues with a Calpha plus nucleic acid residues with
# a C1*
atomsel='Atom CA Protein or Atom C1* NucAcid'

# First snapshot to be analyzed, increase number to ignore an
# equilibration period.
# (By default, md_run.mcr saves snapshots every 25ps, choosing 40 thus
# starts the analysis after 1 nanosecond)
firstsnapshot=0

# No change required below this point
# ===================================

# Do we have a target?
if MacroTarget==''
  RaiseError "This macro requires a target. Either edit the macro file or
  click Options > Macro > Set target to choose a target structure"

Clear
Console Off

# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
  RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water

# We need at least 3 Calpha atoms to superpose
calphas = CountAtom (atomsel)
if calphas<3
  RaiseError 'This macro currently requires at least three residues to
  analyze, because it performs a superposition and RMSD calculation'

ShowMessage "Preparing analysis, please wait..."
Wait 1

# Duplicate the initial object for RMSD calculation
startobj = DuplicateObj (currobj)
# Get a selection of residues that match atomsel in the current and the
start objects
for type in 'curr','start'
    reslist() = ListRes (atomsel) and Obj ((type)obj)
    (type)ressel=join reslist
RemoveObj (startobj)

# Set the summed up RMSDs for CA, Backbone and HeavyAtoms to zero
rmsds=count reslist
for i=1 to 3
    for j=1 to rmsds
        rmsd(i)sum(j)=0.

i=00000+firstsnapshot
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    simtime = Time
    ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
    Wait 1
    # Get per residue RMSDs between current residue selection and start
    residue selection
    AddObj (startobj)
    rmsd1() = SupAtom (atomsel) and Obj (currobj), (atomsel) and Obj
    (startobj),Unit=Res
    rmsd2() = SupAtom Res (currressel) Backbone, Res (startressel)
    Backbone,Unit=Res
    rmsd3() = SupAtom Res (currressel) Element !H, Res (startressel) Element
    !H,Unit=Res
    # Sum up atom positions to calculate RMSFs
    AddPosAtom Res (currressel)
    # Sum up RMSDs
    for j=1 to 3
        for k=1 to rmsds
            rmsd(j)sum(k)=rmsd(j)sum(k)+rmsd(j)(k)
        RemoveObj (startobj)
        # Next snapshot
        i=i+1

if !i
    RaiseError "This macro is meant to analyze a molecular dynamics
trajectory created with md_run, but none was found in this directory"
# Calculate the average
rmsf1list() = RMSFRes (atomsel) and Obj (currobj)
reslist() = ListRes (atomsel) and Obj (currobj),Format='RESNAME RESNUM
MOLNAME'
for j=1 to rmsds
Tabulate
'(reslist(j))', (rmsd(1) sum(j)/i), (rmsd(2) sum(j)/i), (rmsd(3) sum(j)/i), (rmsf
list(j))
# Save table
SaveTab
default, (MacroTarget)_analysisres, Format=Text, Columns=5, NumFormat=%12.3f,_
Residue RMSDs[A]:CA Backbone HeavyAtoms RMSF[A]
HideMessage
MacroTarget (macrotarget)T.sce

# The structure to simulate must be present with a .pdb or .sce extension.
# If a .sce (=YASARA scene) file is present, the cell must have been added.
# You can either set the target structure by clicking on Options > Macro >
# Set target,
# or by uncommenting the line below and specifying it directly.
#MacroTarget = 'c:\MyProject\1crn'

# Extension of the cell on each side of the protein
# '10' means that the cell will be 20 Å larger than the protein
extension=10

# pH at which the simulation should be run, by default physiological pH
ph=7.4

# NaCl concentration in mass percent (0.9% is a physiological solution)
nacl=0.9

# Simulation temperature
# If you run at a temperature that differs from 298K, you also need
# to adapt the pressure control below, look in the PressureCtrl
documentation.
temperature='298K'

# Pressure control mode
# Default: Rescale the cell such that residues named HOH reach a density
# of 0.997 g/l.
# For solvents other than water, you have to create your own solvent box
# as described in the FillCellObj documentation and save it as
#.._solvent.sce.
density=0.997
pressurectrl='SolventProbe, Name=HOH, Density=(density)'

# Alternative: Uncomment below to calculate the pressure from the virial
# and
# rescale the cell to reach a pressure of 1 bar. Use this method if you do not
# know the correct density.
#pressurectrl='Manometer, Pressure=1'

# Constrain bond lengths to hydrogens and water bond angles to allow a
# larger timestep
# If set to 'yes', the MD will run faster, but will be a bit less accurate
# The format used to save the trajectories, sim or xtc
format='sim'

# Duration of the simulation, alternatively use e.g. 'duration=5200' to simulate for 5000 picoseconds
duration=520

# Flag to use a cubic simulation cell. This makes sure that also elongated molecules can rotate freely during very long simulations. If set to 0, the simulation cell will fit the solute more tightly, speeding up the simulation.
cubic=1

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Normally no change required below this point
# ==============================================================

RequireVersion 9.9.25

# Keep the solute from diffusing around and crossing periodic boundaries
CorrectDrift On

# Treat all simulation warnings as errors that stop the macro
WarnIsError On

# Do we have a target?
if MacroTarget==''
   RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to choose a target structure"

Clear
# Do we already have a scene with water or other solvent?
waterscene = FileSize (MacroTarget)_water.sce
solventscene = FileSize (MacroTarget)_solvent.sce
if waterscene
   LoadSce (MacroTarget)_water
elif solventscene
   LoadSce (MacroTarget)_solvent
else
   # No scene with solvent present yet
   # Do we have a scene at all?
scene = FileSize (MacroTarget).sce
if scene
    LoadSce (MacroTarget)
else
    # No scene present, assume it's a PDB or YOB file
    for type in 'pdb','yob','Error'
        size = FileSize (MacroTarget). (type)
        if size
            obj = Load(type) (MacroTarget)
            # Align object with major axes to minimize cell size
            NiceOriObj (obj)
            break
        if type=='Error'
            RaiseError "Initial structure not found. Make sure to create a project directory and place the structure there"
    # Prepare the structure for simulation
    CleanAll
    if Structure
        # Optimize the hydrogen-bonding network (more stable trajectories)
        OptHydAll
        # Create the simulation cell
        Cell Auto, Extension=(extension)
        if cubic
            # And make it cubic, taking the length of the X-axis, which is always the longest
            l = Cell
            Cell (1),(1),(1)
            SaveSce (MacroTarget)
        # Fill with water (always needs periodic boundaries), predict pKas, place counter ions
        Boundary periodic
        Experiment Neutralization
        WaterDensity (density)
        pH (ph)
        NaCl (nacl)
        pKaFile (MacroTarget).pka
        Speed Fast
        Experiment On
        Wait ExpEnd
        # Save scene with water
        SaveSce (MacroTarget) _water
    # Choose timestep and activate constraints
    if constrain=='yes'
        # Constrain bond lengths to hydrogens
        FixBond all, Element H
        # Constrain bond angles in water
        FixAngle Water, Water, Water
        # Multiple timestep: 1.3333 femtoseconds for intramolecular and 3*1.3333 = 4 fs for intermolecular forces
        TimeStep 3, 1.3333
        ts=4
        # Save simulation snapshots every 6250 simulation steps


# (with a timestep of 4 femtoseconds, that's 6540*4 fs = 25 picoseconds).
savesteps=6250
else
# Remove any constraints
FreeBond all,all
FreeAngle all,all,all
# Smaller timestep, since we don't use constraints: 2*1.25 = 2.5 fs
TimeStep 2,1.25
ts=2.5
# Save simulation snapshots every 10000 simulation steps
# (with a timestep of 2.5 femtoseconds, that's 10000*2.5 fs = 25 picoseconds).
savesteps=10000

# Temperature
Temp (temperature)
# Make sure all atoms are free to move
FreeAll
# Already a snapshot/trajectory present?
i=0000
filename='(MacroTarget)(i).(format)'
running = FileSize (filename)
if not running
# Perform energy minimization
Experiment Minimization
Experiment On
Wait ExpEnd
# And now start the real simulation
Sim On
else
# Simulation has been running before
ShowMessage "Simulation has been running before, loading last snapshot..."
Wait 1
# Switch console off to load the snapshots quickly
Console Off
if format=='sim'
# Find and load the last 'sim' snapshot
do
i = i+1
found = FileSize (MacroTarget)(i).sim
while found
i=i-1
LoadSim (MacroTarget)(i)
else
# XTC format requires that the entire trajectory is read in to find the last one
do
i = i+1
eof,time = LoadXTC (filename),(i)
ShowMessage 'Searching XTC trajectory for last snapshot, showing snapshot (i) at (0+time) fs'
Sim Pause
Wait 1
while !eof
    Sim Continue
# Adjust savesteps to save snapshots in the same interval as previously
if i>0
    t = Time
    savesteps=0+t/(ts*i)
    #print 'Time=(t), TimeStep=(ts), savesteps=(savesteps)'
HideMessage

# Set temperature and pressure control
TempCtrl Rescale
PressureCtrl (pressurectrl)

# Uncomment to add distance constraints
# AddSpring O Res Lys 80,H Res Glu 84,Len=1.9

# And finally, make sure that future snapshots are saved
Save(format) (filename),(savesteps)

if duration=='forever'
    Console On
    Wait forever
else
    Console Off
    # Wait for given number of picoseconds
    do
        Wait 10
        t = Time
        while t<duration*1000
            Sim Off

# Number of the object whose RMSDs from the starting conformation will be calculated
# If the protein is an oligomer, check the documentation of the 'Sup' command at 'analyzing a simulation' to avoid pitfalls.
currobj = 1

# Forcefield to use (these are all YASARA commands, so no '=' used)
# Use YASARA2 in YASARA Structure to include a quality Z-score
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# The B-factors calculated from the root-mean-square fluctuations can be too large to fit them
# into the PDB file's B-factor column. Replace e.g. 1.0 with 0.1 to scale
# them down to 10%
bfactorscale=1.0

# Flag to save a PDB file of the solute snapshots for further analysis
pdbsaved=0

# Selection of atoms to include for 'Calpha' RMSD calculation (also
# consider DNA/RNA)
casel='CA Protein or C1* NucAcid'

# Selection of atoms for which the dynamic cross-correlation matrix (DCCM)
# should be visualized.
# Here are some typical examples:
# dccmsel=''                - Don't calculate the DCCM, the default
# dccmsel='Atom CA Protein' - Calculate the DCCM for protein Calpha atoms
# dccmsel='Res Protein'     - Calculate the DCCM for protein residue
# centers
# dccmsel=''             

# Selection of atoms for which the radial distribution function (RDF)
# should be visualized
# Here are some examples:
# rdfsel='' - Don't calculate the DCCM, the default
# rdfsel='O Res HOH,O Res HOH,Bins=40,BinWidth=0.25'
#       - Calculate the RDF of water in 40 bins, each 0.25 A wide (thus
#         up to 10 A).
# rdfsel='CG Res Asp 120,ND1 Res His 200,Bins=20,BinWidth=0.5'
#       - Calculate the RDF between two specific atoms in 20 bins, each
#         0.25 A wide
#       (thus again up to 10 A). Note that you may have to save more
#       snapshots than
#       usually in md_run.mcr to avoid problems with sparse data and
# noisy RDF results.
rdfsel=''  

# First snapshot to be analyzed, increase number to ignore an
# equilibration period.
# (By default, md run.mcr saves snapshots every 25ps, choosing 40 thus
# starts the analysis after 1 nanosecond)
firstsnapshot=0

# No change required below this point
# ===================================

# Do we have a target?
if MacroTarget=''
  RaiseError "This macro requires a target. Either edit the macro file or
  click Options > Macro > Set target to choose a target structure"

Clear
Console Off
# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
  RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water

calphas = CountAtom (casel)
if calphas>0 and calphas<3
  # We cannot superpose 1 or 2 Calpha atoms
casel='None'

ShowMessage "Preparing analysis, please wait..."
Wait 1

# See if structure validation checks should be done (require YASARA2 force field)
checked=0
fof = ForceField
if fof=='YASARA2'
  checked=1

# Duplicate the initial object for RMSD calculation
startobj = DuplicateObj (currobj)
RemoveObj (startobj)

i=00000+firstsnapshot
eimin=1e99
while 1
  # See if next snapshot is present
  sim = FileSize (MacroTarget)(i).sim
  if not sim
    break
  # Yes, load it
  LoadSim (MacroTarget)(i)
  Sim Pause
  # Add time in picoseconds to table
  simtime = Time
  ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
  Wait 1
  Tabulate (simtime/1000)
  # Get energy components, including packing energies for YASARA2 force field
  if checked
    ebindlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i),packing1,packing3 = EnergyAll All
  else
    ebindlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i) = EnergyAll All
    packing1=0
    packing3=0
elist(i) =
 ebndlist(i)+eanglist(i)+edihlist(i)+eplnlist(i)+ecoulist(i)+evdwlist(i)+packing1+packing3

# The following examples provide a few hints for other things to analyze.
# If you uncomment one of the examples, keep in mind that every value you
# tabulate becomes an additional column in the table, so you must increase the
# 'Columns' parameter of the SaveTab command further below (and the table
# header will also no longer indicate the proper results unless you adapt it).
#
# Example: Measure the distance between the carboxyl group of Glu 123 (Cdelta)
#          and the guanidinium group of Arg 345 (Czeta):
# Tabulate Distance CD Res Glu 123, CZ Res Arg 345
#
# Example: Measure the distance between two centers of mass, e.g. the loop from
#          residue Ala 205 to Glu 210, and the ligand NAD:
# cenA() = GroupCenter Res Ala 205 - Glu 210, Type=Mass
# cenB() = GroupCenter Res NAD, Type=Mass
# Tabulate (norm (cenA-cenB))
#
# Example: Check if the carboxyl group of Glu 123 and the guanidinium group of
#          Arg 345 are currently hydrogen-bonded (1) or not (0):
# hbolist() = ListHBoAtom Sidechain Res Glu 123, Sidechain Res Arg 345
# Tabulate (count hbolist>0)
#
# Example: Count the number of atoms in molecule A that are hydrogen bonded to B
# hbolist() = ListHBoAtom Mol A,Mol B
# Tabulate (count hbolist)
#
# Example: Calculate the current potential energy of residue Glu 123:
# Tabulate EnergyRes Glu 123
#
# Example: Calculate the backbone RMSD for residues 1-120:
# Tabulate SupAtom Backbone Res 1-120 Obj (currobj),Backbone Res 1-120 Obj (startobj)
#
# Save the minimum energy structure (ignoring solvent-solvent interactions)
e = EnergyObj (currobj)
if checked
    # Calculate structure validation Z-scores, using the formula from homology modeling
    for type in 'dihedrals','packing1d','packing3d'
        zscore(type) = CheckObj (currobj), (type)
zscorelist(i)=zscoredihedrals*0.145+zscorepacking1d*0.390+zscorepacking3d*0.465
if rdfsel=''
    # Collect data for radial distribution function
    BinDistance (rdfsel)
    Sim Off
if e<emin
    emin=e
    SaveSce (MacroTarget)_energymin
if pdocsaved
    # Save a PDB file of the solute
    SavePDB (currobj),(MacroTarget)_(i)
    # Add CA, backbone and heavy atom RMSDs to table
    AddObj (startobj)
    # Trick: If the solute object contains neither CA nor backbone atoms, # we simply assign the SupAtom error code (=0)
    carmsdlist(i) = SupAtom (casel) and Obj (currobj),(casel) and Obj (startobj)
    bbrmsdlist(i) = SupAtom Backbone Obj (currobj),Backbone Obj (startobj)
    aarmsdlist(i) = SupAtom Element !H Obj (currobj),Element !H Obj (startobj)
    # Add results to table
    Tabulate (elist(i)),(ebndlist(i)),(eanglist(i)),(edihlist(i)),(eplnlist(i)),(ecoulist(i)),(evdwlstlist(i)),(carmsdlist(i)),(bbrmsdlist(i)),(aarmsdlist(i))
    if checked
        Tabulate (zscorelist(i))
        # Add the current atom positions to internal table to obtain RMSF and average positions
        AddPosAtom Obj (currobj)
        RemoveObj (startobj)
        # Next snapshot
        i=i+1
if !i
    RaiseError "This macro is meant to analyze a molecular dynamics trajectory created with md_run, but none was found in this directory"

    # Add average results to table
    Tabulate 'Average',(mean elist),(mean ebndlist),(mean eanglist),(mean edihlist),(mean eplnlist),
    (mean ecoulist),(mean evdwlstlist),(mean carmsdlist),(mean bbrmsdlist),(mean aarmsdlist)
    header='____Time[ps] Energy[(EnergyUnit)]____Bond _______Angle ______Dihedral ___Planarity _____Coulomb _________VdW _RMSDs[A]:CA ______Backbone__HeavyAtoms'
    if checked
        header=header+' QualityScore'
        Tabulate (mean zscorelist)
    # Save main analysis table
SaveTab
default,(MacroTarget)_analysis,Format=Text,Columns=(11+checked),NumFormat=12.3f,(header)

# Calculate time-average structure and set B-factors according to RMSF
AveragePosAtom Obj (currobj)
RMSFAAtom Obj (currobj),Unit=BFactor
if bfactorscale!=1.0
    # Scale B-factors so that they fit into the PDB format
    first,last=SpanAtom Obj (currobj)
    for i=first to last
        bf=BFactorAtom (i)
        BFactorAtom (i),(bf*bfactorscale)
# The time average structure has incorrect covalent geometry and should be energy minimized
SavePDB (currobj),(MacroTarget)_average

""
# Example: Create an additional RMSF file, in case B-factors are too large for the PDB format
DelTab default
first,last = SpanAtom Obj (currobj)
rmsflist() = RMSFAAtom Obj (currobj)
for i=first to last
    res = ListAtom (i),Format='RESNAME,RESNUM'
    Tabulate (i),(res),(rmsflist(i-first+1))
SaveTab
default,(MacroTarget)_rmsf,Format=Text,Columns=4,NumFormat=8.2f,"RMSF Table"
""
if rdfsel!=''
    # Additionally calculate and show the radial distribution function (RDF).
    MakeTab RDF,Dimensions=1
    Tabulate RDF
    SaveTab RDF,(MacroTarget)_rdf,Format=Text,Columns=1,NumFormat=6.3f,
        'Radial distribution function with parameters (rdfsel)'
    obj = ShowTab RDF,Width=1.0,Range=10,MinCol=Blue,MaxCol=Yellow
    PosObj (obj),X=0,Y=-12,Z=31
    RotateObj (obj),X=-90
    SaveSce (MacroTarget)_rdf
    DelObj (obj)
if dccmsel!=''
    # Additionally calculate and show the dynamic cross-correlation matrix (DCCM).
    # This matrix correlates the displacements from the time average structure,
    # see the documentation of the 'DCCM' command for details.
    # First get the number of selected units, i.e. the rows/columns in the matrix
    units = Count(dccmsel)
    if !units
RaiseError 'The DCCM selection (dccmsel) did not match any atoms'
# Take the time average structure as the start object to superpose onto
DelObj (startobj)
startobj = DuplicateObj (currobj)
RemoveObj (startobj)
# Loop over the snapshots a second time to calculate the displacements
from the time average
i=00000+firstsnapshot
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    ShowMessage 'Calculating dynamic cross-correlation matrix, analyzing
snapshot (0+i)...'
    Wait 1
    Sim Off
    # Superpose snapshot on the time average structure
    AddObj (startobj)
    SupAtom (casel) and Obj (currobj), (casel) and Obj (startobj)
    # Add the current displacements to an internal table to obtain the
DCCM
    AddDisp(dccmsel) Obj (currobj), (dccmsel) Obj (startobj)
    RemoveObj (startobj)
    # Next snapshot
    i=i+1
    # Store the DCCM in a table
    MakeTab DCCM,Dimensions=2,Columns=(units)
    Tabulate DCCM
    # Visualize the DCCM
    pointwidth=1.
    height=5.
    dccmobj1 = ShowTab DCCM,Width=(pointwidth),Range=(height),Min=-1,Max=1.0
    # By default, ShowTab shows the minimum at Z=0, move so that correlation
0 is at Z=0
    MoveObj (dccmobj1), Z=(height*0.5)
    # Visualize the zero level with a flat DCCM wireframe
    dccmobj2 = ShowTab DCCM,Width=(pointwidth),Range=0,Min=-1,Max=1.0
    dccmobj3 = ShowWireObj (dccmobj2), Static, Mesh=Solid
    DelObj (dccmobj2)
    PointPar Radius=0.5, Plastic=No
    NameObj (dccmobj3), ZeroLevel
    RotateObj (dccmobj1) (dccmobj3), X=180
    # Create a text object with the residue names and the table header
    textwidth=pointwidth*units*2
    textobj1 = MakeTextObj Units, Width=(textwidth), Height=(textwidth)
    Font Arial, Height=(pointwidth*0.6), Color=Yellow, Depth=0.5, DepthCol=Red
    idlist() = List(dccmsel) Obj (currobj), Format='MOLNAME RESName RESNUM'
    for i=1 to units
        PosText X=(textwidth*0.5+pointwidth*-0.5*(units+6)),
        Y=(textwidth*0.5+pointwidth*(0.5*units-i)), justify=left
Print (idlist(i))
# Duplicate the labels at the bottom
textobj2 = DuplicateObj (textobj1)
RotateObj (textobj2),Z=90
DelObj not (dccmobj1) (dccmobj3) (join textobj)
RenumberObj all
# Save the matrix
SaveTab
DCCM,(MacroTarget)_dccm,Format=Text,Columns=(units),NumFormat=6.3f,
'Dynamic Cross-Correlation Matrix for (units) selected units'
# Save the visualized matrix
SaveSce (MacroTarget)_dccm
HideMessage

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Consider protein residues with a Calpha plus nucleic acid residues with
# a C1*
atomsel='Atom CA Protein or Atom C1* NucAcid'

# First snapshot to be analyzed, increase number to ignore an
# equilibration period.
# (By default, md_run.mcr saves snapshots every 25ps, choosing 40 thus
# starts the analysis after 1 nanosecond)
firstsnapshot=0

# No change required below this point
# ===================================

# Do we have a target?
if MacroTarget==''
    RaiseError "This macro requires a target. Either edit the macro file or
    click Options > Macro > Set target to choose a target structure"

Clear
Console Off
# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
    RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water
# We need at least 3 Calpha atoms to superpose
calphas = CountAtom (atomsel)
if calphas<3
    RaiseError 'This macro currently requires at least three residues to
analyze, because it performs a superposition and RMSD calculation'

ShowMessage "Preparing analysis, please wait..."
Wait 1

# Duplicate the intial object for RMSD calculation
startobj = DuplicateObj (currobj)

# Get a selection of residues that match atomsel in the current and the
start objects
for type in 'curr','start'
    reslist() = ListRes (atomsel) and Obj ((type)obj)
    (type)ressel=join reslist
RemoveObj (startobj)

# Set the summed up RMSDs for CA, BackBone and HeavyAtoms to zero
rmsds=count reslist
for i=1 to 3
    for j=1 to rmsds
        rmsd(i)sum(j)=0.

i=00000+firstsnapshot
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    simtime = Time
    ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
    Wait 1
    # Get per residue RMSDs between current residue selection and start
residue selection
    AddObj (startobj)
    rmsd1() = SupAtom (atomsel) and Obj (currobj), (atomsel) and Obj
    (startobj),Unit=Res
    rmsd2() = SupAtom Res (currressel) Backbone, Res (startressel)
    Backbone,Unit=Res
    rmsd3() = SupAtom Res (currressel) Element !H, Res (startressel) Element
    !H,Unit=Res
    # Sum up atom positions to calculate RMSFs
    AddPosAtom Res (currressel)
    # Sum up RMSDs
    for j=1 to 3
        for k=1 to rmsds
            rmsd(j)sum(k)=rmsd(j)sum(k)+rmsd(j)(k)
RemoveObj (startobj)
    # Next snapshot
i=i+1

if !i
    RaiseError "This macro is meant to analyze a molecular dynamics
trajectory created with md_run, but none was found in this directory"
# Calculate the average
rmsflist() = RMSFRes (atomsel) and Obj (currobj)
reslist() = ListRes (atomsel) and Obj (currobj),Format='RESNAME RESNUM'
for j=1 to rmsds
    Tabulate
    
    '(reslist(j))',(rmsd(1)sum(j)/i),(rmsd(2)sum(j)/i),(rmsd(3)sum(j)/i),(rmsf
    list(j))
    
    # Save table
    SaveTab
    default,(MacroTarget)_analysisres,Format=Text,Columns=5,NumFormat=%12.3f,
    Residue _RMSDs[A]:CA _Backbone _HeavyAtoms______RMSF[A]

# The structure to simulate must be present with a .pdb or .sce extension. # If a .sce (=YASARA scene) file is present, the cell must have been added. # You can either set the target structure by clicking on Options > Macro > Set target, # or by uncommenting the line below and specifying it directly. #MacroTarget = 'c:\MyProject\1crn' # Extension of the cell on each side of the protein # '10' means that the cell will be 20 A larger than the protein extension=10

# pH at which the simulation should be run, by default physiological pH ph=7.4

# NaCl concentration in mass percent (0.9% is a physiological solution) nacl=0.9

# Simulation temperature # If you run at a temperature that differs from 298K, you also need # to adapt the pressure control below, look in the PressureCtrl documentation. temperature='298K'

# Pressure control mode # Default: Rescale the cell such that residues named HOH reach a density of 0.997 g/l. # For solvents other than water, you have to create your own solvent box # as described in the FillCellObj documentation and save it as .._solvent.sce. density=0.997 pressurectrl='SolventProbe,Name=HOH,Density=(density)'


# Alternative: Uncomment below to calculate the pressure from the virial and
# rescale the cell to reach a pressure of 1 bar. Use this method if you do not
# know the correct density.
#pressurectrl='Manometer,Pressure=1'

# Constrain bond lengths to hydrogens and water bond angles to allow a larger timestep
# If set to 'yes', the MD will run faster, but will be a bit less accurate
constrain='no'

# The format used to save the trajectories, sim or xtc
format='sim'

duration=520

# Flag to use a cubic simulation cell. This makes sure that also elongated molecules can rotate freely during very long simulations. If set to 0, the simulation cell will fit the solute more tightly, speeding up the simulation.
cubic=1

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Normally no change required below this point
# ================================================================

RequireVersion 9.9.25

# Keep the solute from diffusing around and crossing periodic boundaries
CorrectDrift On

# Treat all simulation warnings as errors that stop the macro
WarnIsError On

# Do we have a target?
if MacroTarget==''
    RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to choose a target structure"

Clear
# Do we already have a scene with water or other solvent?
waterscene = FileSize (MacroTarget)_water.sce
solventscene = FileSize (MacroTarget)_solvent.sce
if waterscene
    LoadSce (MacroTarget)_water
elif solventscene
    LoadSce (MacroTarget)_solvent
else
    # No scene with solvent present yet
    # Do we have a scene at all?
    scene = FileSize (MacroTarget).sce
    if scene
        LoadSce (MacroTarget)
    else
        # No scene present, assume it's a PDB or YOB file
        for type in 'pdb','yob','Error'
            size = FileSize (MacroTarget).(type)
            if size
                obj = Load(type) (MacroTarget)
                # Align object with major axes to minimize cell size
                NiceOriObj (obj)
                break
        if type=='Error'
            RaiseError "Initial structure not found. Make sure to create a
            project directory and place the structure there"
        # Prepare the structure for simulation
        CleanAll
        if Structure
            # Optimize the hydrogen-bonding network (more stable trajectories)
            OptHydAll
            # Create the simulation cell
            Cell Auto,Extension=(extension)
            if cubic
                # And make it cubic, taking the length of the X-axis, which is
                # always the longest
                l = Cell
                Cell (l),(l),(l)
                SaveSce (MacroTarget)
        # Fill with water (always needs periodic boundaries), predict pKas,
        place counter ions
        Boundary periodic
        Experiment Neutralization
        WaterDensity (density)
        pH (ph)
        NaCl (nacl)
        pKaFile (MacroTarget).pka
        Speed Fast
        Experiment On
        Wait ExpEnd
        # Save scene with water
        SaveSce (MacroTarget)_water

        # Choose timestep and activate constraints
        if constrain=='yes'
# Constrain bond lengths to hydrogens
FixBond all,Element H
# Constrain bond angles in water
FixAngle Water,Water,Water
# Multiple timestep: 1.3333 femtoseconds for intramolecular and 3*1.3333 = 4 fs for intermolecular forces
TimeStep 3,1.3333
ts=4
# Save simulation snapshots every 6250 simulation steps
# (with a timestep of 4 femtoseconds, that's 6540*4 fs = 25 picoseconds).
savesteps=6250
else
    # Remove any constraints
    FreeBond all,all
    FreeAngle all,all,all
    # Smaller timestep, since we don't use constraints: 2*1.25 = 2.5 fs
    TimeStep 2,1.25
ts=2.5
    # Save simulation snapshots every 10000 simulation steps
    # (with a timestep of 2.5 femtoseconds, that's 10000*2.5 fs = 25 picoseconds).
savesteps=10000
# Temperature
Temp (temperature)
# Make sure all atoms are free to move
FreeAll
# Already a snapshot/trajectory present?
i=00000
filename='(MacroTarget)(i).format'
running = FileSize (filename)
if not running
    # Perform energy minimization
    Experiment Minimization
    Experiment On
    Wait ExpEnd
    # And now start the real simulation
    Sim On
else
    # Simulation has been running before
    ShowMessage "Simulation has been running before, loading last snapshot..."
    Wait 1
    # Switch console off to load the snapshots quickly
    Console Off
    if format=='sim'
        # Find and load the last 'sim' snapshot
        do
            i = i+1
            found = FileSize (MacroTarget)(i).sim
            while found
                i=i-1
            LoadSim (MacroTarget)(i)
else
    # XTC format requires that the entire trajectory is read in to find
    # the last one
    do
        i = i+1
        eof, time = LoadXTC (filename),(i)
        ShowMessage 'Searching XTC trajectory for last snapshot, showing
        snapshot (i) at (0+time) fs'
        Sim Pause
        Wait 1
        while !eof
            Sim Continue
            # Adjust savesteps to save snapshots in the same interval as previously
            if i>0
                t = Time
                savesteps=0+t/(ts*i)
                #print 'Time=(t), TimeStep=(ts), savesteps=(savesteps)'
            HideMessage
            # Set temperature and pressure control
            TempCtrl Rescale
            PressureCtrl (pressurectrl)

            # Uncomment to add distance constraints
            # AddSpring O Res Lys 80, H Res Glu 84, Len=1.9

            # And finally, make sure that future snapshots are saved
            Save(format) (filename),(savesteps)

            if duration=='forever'
                Console On
                Wait forever
            else
                Console Off
                # Wait for given number of picoseconds
                do
                    Wait 10
                    t = Time
                    while t<duration*1000
                    Sim Off

    # Number of the object whose RMSDs from the starting conformation will be
    # calculated
    # If the protein is an oligomer, check the documentation of the 'Sup'
    # command at 'analyzing a simulation' to avoid pitfalls.
    currobj = 1

    # Forcefield to use (these are all YASARA commands, so no '=' used)
    # Use YASARA2 in YASARA Structure to include a quality Z-score
    ForceField AMBER03

    # Cutoff
    Cutoff 7.86
# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# The B-factors calculated from the root-mean-square fluctuations can be
too large to fit them
# into the PDB file's B-factor column. Replace e.g. 1.0 with 0.1 to scale
# them down to 10%
bfactorscale=1.0

# Flag to save a PDB file of the solute snapshots for further analysis
pdsaved=0

# Selection of atoms to include for 'Calpha' RMSD calculation (also
# consider DNA/RNA)
casel='CA Protein or Cl* NucAcid'

# Selection of atoms for which the dynamic cross-correlation matrix (DCCM)
# should be visualized.
# Here are some typical examples:
# dccmsel='' - Don't calculate the DCCM, the default
# dccmsel='Atom CA Protein' - Calculate the DCCM for protein Calpha atoms
# dccmsel='Res Protein' - Calculate the DCCM for protein residue
# centers
dccmsel=''

# Selection of atoms for which the radial distribution function (RDF)
# should be visualized
# Here are some examples:
# rdfsel='' - Don't calculate the RDF, the default
# rdfsel='O Res HOH,O Res HOH,Bins=40,BinWidth=0.25'
# - Calculate the RDF of water in 40 bins, each 0.25 A wide (thus
#   up to 10 A).
# rdfsel='CG Res Asp 120,ND1 Res His 200,Bins=20,BinWidth=0.5'
# - Calculate the RDF between two specific atoms in 20 bins, each
#   0.25 A wide
#   (thus again up to 10 A). Note that you may have to save more
#   snapshots than
#   usually in md_run.mcr to avoid problems with sparse data and
#   noisy RDF results.
rdfsel=''

# First snapshot to be analyzed, increase number to ignore an
# equilibration period.
# (By default, md_run.mcr saves snapshots every 25ps, choosing 40 thus
# starts the analysis after 1 nanosecond)
firstsnapshot=0

# No change required below this point
# ===================================
# Do we have a target?
if MacroTarget==''
    RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to choose a target structure"

Clear
Console Off
# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
    RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water

calphas = CountAtom (casel)
if calphas>0 and calphas<3
    # We cannot superpose 1 or 2 Calpha atoms
casel='None'

ShowMessage "Preparing analysis, please wait..."
Wait 1

# See if structure validation checks should be done (require YASARA2 force field)
checked=0
fof = ForceField
if fof=='YASARA2'
    checked=1

# Duplicate the intial object for RMSD calculation
startobj = DuplicateObj (currobj)
RemoveObj (startobj)

i=00000+firstsnapshot
emin=1e99
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    # Add time in picoseconds to table
    simtime = Time
    ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
    Wait 1
    Tabulate (simtime/1000)
    # Get energy components, including packing energies for YASARA2 force field
    if checked
ebndlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i),pack1,packing3 = EnergyAll All
else

ebndlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i) = EnergyAll All
    packing1=0
    packing3=0
    elist(i) =
    ebndlist(i)+eanglist(i)+edihlist(i)+eplnlist(i)+ecoulist(i)+evdwlist(i)+pack1+packing3

# The following examples provide a few hints for other things to analyze.
# If you uncomment one of the examples, keep in mind that every value you
# tabulate becomes an additional column in the table, so you must increase the
# 'Columns' parameter of the SaveTab command further below (and the
# table
# header will also no longer indicate the proper results unless you
# adapt it).

# Example: Measure the distance between the carboxyl group of Glu 123 (Cdelta)
# and the guanidinium group of Arg 345 (Czeta):
# Tabulate Distance CD Res Glu 123, CZ Res Arg 345
#
# Example: Measure the distance between two centers of mass, e.g. the loop from
# residue Ala 205 to Glu 210, and the ligand NAD:
# cenA() = GroupCenter Res Ala 205 - Glu 210, Type=Mass
# cenB() = GroupCenter Res NAD, Type=Mass
# Tabulate (norm (cenA-cenB))
#
# Example: Check if the carboxyl group of Glu 123 and the guanidinium group of
# Arg 345 are currently hydrogen-bonded (1) or not (0):
# hbolist() = ListHBoAtom Sidechain Res Glu 123, Sidechain Res Arg 345
# Tabulate (count hbolist>0)
#
# Example: Count the number of atoms in molecule A that are hydrogen
# bonded to B
# hbolist() = ListHBoAtom Mol A,Mol B
# Tabulate (count hbolist)
#
# Example: Calculate the current potential energy of residue Glu 123:
# Tabulate EnergyRes Glu 123
#
# Example: Calculate the backbone RMSD for residues 1-120:
# Tabulate SupAtom Backbone Res 1-120 Obj (currobj), Backbone Res 1-120 Obj (startobj)
#
# Save the minimum energy structure (ignoring solvent-solvent interactions)

e = EnergyObj (currobj)
if checked
    # Calculate structure validation Z-scores, using the formula from homology modeling
    for type in 'dihedrals','packing1d','packing3d'
        zscore(type) = CheckObj (currobj), (type)

zscorelist(i) = zscoredihedrals*0.145+zscorepacking1d*0.390+zscorepacking3d*0.465
if rdfsel!=''
    # Collect data for radial distribution function
    BinDistance (rdfsel)
    Sim Off
if e<emin
    emin=e
    SaveSce (MacroTarget)_energymin
if pdbsaved
    # Save a PDB file of the solute
    SavePDB (currobj), (MacroTarget)_(i)
    # Add CA, backbone and heavy atom RMSDs to table
    AddObj (startobj)
    # Trick: If the solute object contains neither CA nor backbone atoms, # we simply assign the SupAtom error code (=0)
    carmsdlist(i) = SupAtom (casel) and Obj (currobj), (casel) and Obj (startobj)
    bbrmsdlist(i) = SupAtom Backbone Obj (currobj), Backbone Obj (startobj)
    aarmsdlist(i) = SupAtom Element !H Obj (currobj), Element !H Obj (startobj)
    # Add results to table
    Tabulate
    (elist(i)), (ebndlist(i)), (eanglist(i)), (edihlist(i)), (eplnlist(i)), (ecoulist(i)), (evdwlist(i)),
    (carmisdlist(i)), (bbrmsdlist(i)), (aarmsdlist(i))
if checked
    Tabulate (zscorelist(i))
    # Add the current atom positions to internal table to obtain RMSF and average positions
    AddPosAtom Obj (currobj)
    RemoveObj (startobj)
    # Next snapshot
    i=i+1
if !i
    RaiseError "This macro is meant to analyze a molecular dynamics trajectory created with md_run, but none was found in this directory"

    # Add average results to table
    Tabulate 'Average', (mean elist), (mean ebndlist), (mean eanglist), (mean edihlist), (mean eplnlist),
    (mean ecoulist), (mean evdwlist), (mean carmsdlist), (mean bbrmsdlist), (mean aarmsdlist)
header='Time[ps] Energy[(EnergyUnit)] Bond Angle
Dihedral Planarity Coulomb VdW RMSDs[Å]:CA
Backbone HeavyAtoms'
if checked
    header=header+' QualityScore'
Tabulate (mean zscorelist)
# Save main analysis table
SaveTab
default,(MacroTarget)_analysis,Format=Text,Columns=(11+checked),NumFormat=12.3f,(header)

# Calculate time-average structure and set B-factors according to RMSF
AveragePosAtom Obj (currobj)
RMSFAtom Obj (currobj),Unit=BFactor
if bfactorscale!=1.0
    # Scale B-factors so that they fit into the PDB format
    first,last=SpanAtom Obj (currobj)
    for i=first to last
        bf=BFactorAtom (i)
        BFactorAtom (i),(bf*bfactorscale)
# The time average structure has incorrect covalent geometry and should be
energy minimized
SavePDB (currobj),(MacroTarget)_average

"""
# Example: Create an additional RMSF file, in case B-factors are too large
for the PDB format
DelTab default
first,last=SpanAtom Obj (currobj)
rmsflist() = RMSFAtom Obj (currobj)
for i=first to last
    res = ListAtom (i),Format='RESNAME,RESNUM'
    Tabulate (i),(res),(rmsflist(i-first+1))
SaveTab
default,(MacroTarget)_rmsf,Format=Text,Columns=4,NumFormat=8.2f,"RMSF Table"
"""
if rdfsel!=''
    # Additionally calculate and show the radial distribution function
    (RDF).
    MakeTab RDF,Dimensions=1
    Tabulate RDF
    SaveTab RDF,(MacroTarget)_rdf,Format=Text,Columns=1,NumFormat=6.3f,
    'Radial distribution function with parameters (rdfsel)'
    obj = ShowTab RDF,Width=1.0,Range=10,MinCol=Blue,MaxCol=Yellow
    PosObj (obj),X=0,Y=-12,Z=31
    RotateObj (obj),X=-90
    SaveSce (MacroTarget)_rdf
    DelObj (obj)
if dccmse1!=''
    # Additionally calculate and show the dynamic cross-correlation matrix
    (DCCM).
# This matrix correlates the displacements from the time average structure,
# see the documentation of the 'DCCM' command for details.
# First get the number of selected units, i.e. the rows/columns in the matrix
units = Count(dccmsel)
if !units
   RaiseError 'The DCCM selection (dccmsel) did not match any atoms'
# Take the time average structure as the start object to superpose onto
DelObj (startobj)
startobj = DuplicateObj (currobj)
RemoveObj (startobj)
# Loop over the snapshots a second time to calculate the displacements from the time average
i=00000+firstsnapshot
while 1
   # See if next snapshot is present
   sim = FileSize (MacroTarget)(i).sim
   if not sim
      break
   # Yes, load it
   LoadSim (MacroTarget)(i)
   Sim Pause
   ShowMessage 'Calculating dynamic cross-correlation matrix, analyzing snapshot (0+i)...
   Wait 1
   Sim Off
   # Superpose snapshot on the time average structure
   AddObj (startobj)
   SupAtom (casel) and Obj (currobj),(casel) and Obj (startobj)
   # Add the current displacements to an internal table to obtain the DCCM
   AddDisp(dccmsel) Obj (currobj),(dccmsel) Obj (startobj)
   RemoveObj (startobj)
   # Next snapshot
   i=i+1
# Store the DCCM in a table
MakeTab DCCM,Dimensions=2,Columns=(units)
Tabulate DCCM
# Visualize the DCCM
pointwidth=1.
height=5.
dccmobj1 = ShowTab DCCM,Width=(pointwidth),Range=(height),Min=-1,Max=1.0
# By default, ShowTab shows the minimum at Z=0, move so that correlation 0 is at Z=0
MoveObj (dccmobj1),Z=(height*0.5)
# Visualize the zero level with a flat DCCM wireframe
dccmobj2 = ShowTab DCCM,Width=(pointwidth),Range=0,Min=-1,Max=1.0
dccmobj3 = ShowWireObj (dccmobj2),Static,Mesh=Solid
DelObj (dccmobj2)
PointPar Radius=0.5,Plastic=No
NameObj (dccmobj3),ZeroLevel
RotateObj (dccmobj1) (dccmobj3),X=180
# Create a text object with the residue names and the table header
textwidth=pointwidth*units*2
textobj1 = MakeTextObj Units,Width=(textwidth),Height=(textwidth)
Font Arial,Height=(pointwidth*0.6),Color=Yellow,Depth=0.5,DepthCol=Red
idlist() = List(dccmsel) Obj (currobj),Format='MOLNAME RESName RESNUM'
for i=1 to units
   PosText X=(textwidth*0.5+pointwidth*-0.5*(units+6)),
   Y=(textwidth*0.5+pointwidth*(0.5*units-i)),justify=left
   Print (idlist(i))
# Duplicate the labels at the bottom
textobj2 = DuplicateObj (textobj1)
RotateObj (textobj2),Z=90
DelObj not (dccmobj1) (dccmobj3) (join textobj)
RenumberObj all
# Save the matrix
SaveTab
DCCM,(MacroTarget)_dccm,Format=Text,Columns=(units),NumFormat=6.3f,
   'Dynamic Cross-Correlation Matrix for (units) selected units'
# Save the visualized matrix
SaveSce (MacroTarget)_dccm
HideMessage

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Consider protein residues with a Calpha plus nucleic acid residues with
a C1*
atomsel='Atom CA Protein or Atom C1* NucAcid'

# First snapshot to be analyzed, increase number to ignore an
equilibration period.
# (By default, md_run.mcr saves snapshots every 25ps, choosing 40 thus
starts the analysis after 1 nanosecond)
firstsnapshot=0

# No change required below this point
# ===================================
# Do we have a target?
if MacroTarget==''
   RaiseError "This macro requires a target. Either edit the macro file or
   click Options > Macro > Set target to choose a target structure"
Clear
Console Off
# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
    RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water

# We need at least 3 Calpha atoms to superpose
calphas = CountAtom (atomsel)
if calphas<3
    RaiseError 'This macro currently requires at least three residues to analyze, because it performs a superposition and RMSD calculation'

ShowMessage "Preparing analysis, please wait..."
Wait 1

# Duplicate the initial object for RMSD calculation
startobj = DuplicateObj (currobj)

# Get a selection of residues that match atomsel in the current and the start objects
for type in 'curr','start'
    reslist() = ListRes (atomsel) and Obj ((type)obj)
    (type)ressel=join reslist
RemoveObj (startobj)

# Set the summed up RMSDs for CA, Backbone and HeavyAtoms to zero
rmsds=count reslist
for i=1 to 3
    for j=1 to rmsds
        rmsd(i)sum(j)=0.

i=00000+firstsnapshot
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    simtime = Time
    ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
    Wait 1
    # Get per residue RMSDs between current residue selection and start residue selection
    AddObj (startobj)
    rmsd1() = SupAtom (atomsel) and Obj (currobj), (atomsel) and Obj (startobj),Unit=Res
    rmsd2() = SupAtom Res (currressel) Backbone, Res (startressel) Backbone,Unit=Res
    # Sum up atom positions to calculate RMSFs
AddPosAtom Res (currressel)
# Sum up RMSDs
for j=1 to 3
  for k=1 to rmsds
    rmsd(j)sum(k)=rmsd(j)sum(k)+rmsd(j)(k)
  RemoveObj (startobj)
# Next snapshot
  i=i+1
if !i
  RaiseError "This macro is meant to analyze a molecular dynamics trajectory created with md_run, but none was found in this directory"
# Calculate the average
rmsflist() = RMSFRes (atomsel) and Obj (currobj)
reslist() = ListRes (atomsel) and Obj (currobj),Format='RESNAME RESNUM MOLNAME'
for j=1 to rmsds
  Tabulate
    '(reslist(j))', (rmsd(1)sum(j)/i),(rmsd(2)sum(j)/i),(rmsd(3)sum(j)/i),(rmsf
list(j))
  # Save table
  SaveTab
  default,(MacroTarget)_analysisres,Format=Text,Columns=5,NumFormat=%12.3f,_
  _Residue _RMSDs[A]:CA ____Backbone __HeavyAtoms______RMSF[A]
HideMessage
MacroTarget (macrotarget)C.sce

# The structure to simulate must be present with a .pdb or .sce extension.
# If a .sce (=YASARA scene) file is present, the cell must have been added.
# You can either set the target structure by clicking on Options > Macro > Set target,
# or by uncommenting the line below and specifying it directly.
#MacroTarget = 'c:\MyProject\1crn'

# Extension of the cell on each side of the protein
# '10' means that the cell will be 20 A larger than the protein
extension=10

# pH at which the simulation should be run, by default physiological pH
ph=7.4

# NaCl concentration in mass percent (0.9% is a physiological solution)
nacl=0.9

# Simulation temperature
# If you run at a temperature that differs from 298K, you also need
# to adapt the pressure control below, look in the PressureCtrl documentation.
temperature='298K'

# Pressure control mode
# Default: Rescale the cell such that residues named HOH reach a density of 0.997 g/l.
# For solvents other than water, you have to create your own solvent box
# as described in the FillCellObj documentation and save it as
# .._solvent.sce.

density=0.997
pressurectrl='SolventProbe,Name=HOH,Density=(density)'

# Alternative: Uncomment below to calculate the pressure from the virial
# and rescale the cell to reach a pressure of 1 bar. Use this method if you do not
# know the correct density.
#pressurectrl='Manometer,Pressure=1'

# Constrain bond lengths to hydrogens and water bond angles to allow a larger timestep
# If set to 'yes', the MD will run faster, but will be a bit less accurate
constrain='no'

# The format used to save the trajectories, sim or xtc
format='sim'

duration=520

cubic=1

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

CutOff
CutOff 7.86

Boundary periodic

Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Normally no change required below this point
RequireVersion 9.9.25

# Keep the solute from diffusing around and crossing periodic boundaries
CorrectDrift On

# Treat all simulation warnings as errors that stop the macro
WarnIsError On

# Do we have a target?
if MacroTarget==''
    RaiseError "This macro requires a target. Either edit the macro file or
    click Options > Macro > Set target to choose a target structure"

Clear
# Do we already have a scene with water or other solvent?
waterscene = FileSize (MacroTarget)_water.sce
solventscene = FileSize (MacroTarget)_solvent.sce
if waterscene
    LoadSce (MacroTarget)_water
elif solventscene
    LoadSce (MacroTarget)_solvent
else
    # No scene with solvent present yet
    # Do we have a scene at all?
    scene = FileSize (MacroTarget).sce
    if scene
        LoadSce (MacroTarget)
    else
        # No scene present, assume it's a PDB or YOB file
        for type in 'pdb','yob','Error'
            size = FileSize (MacroTarget).(type)
            if size
                obj = Load(type) (MacroTarget)
                # Align object with major axes to minimize cell size
                NiceOriObj (obj)
                break
        if type=='Error'
            RaiseError "Initial structure not found. Make sure to create a
            project directory and place the structure there"
    # Prepare the structure for simulation
    CleanAll
    if Structure
        # Optimize the hydrogen-bonding network (more stable trajectories)
        OptHydAll
        # Create the simulation cell
        Cell Auto,Extension=(extension)
        if cubic
            # And make it cubic, taking the length of the X-axis, which is
            always the longest
            l = Cell
            Cell (1),(1),(1)
        SaveSce (MacroTarget)
        # Fill with water (always needs periodic boundaries), predict pKas,
        place counter ions
        Boundary periodic
        Experiment Neutralization
        WaterDensity (density)
        pH (ph)
        NaCl (nacl)
        pKaFile (MacroTarget).pka
Speed Fast
Experiment On
Wait ExpEnd
# Save scene with water
SaveSce (MacroTarget)_water

# Choose timestep and activate constraints
if constrain=='yes'
  # Constrain bond lengths to hydrogens
  FixBond all,Element H
  # Constrain bond angles in water
  FixAngle Water,Water,Water
  # Multiple timestep: 1.3333 femtoseconds for intramolecular and 3*1.3333
  = 4 fs for intermolecular forces
  TimeStep 3,1.3333
  ts=4
  # Save simulation snapshots every 6250 simulation steps
  # (with a timestep of 4 femtoseconds, that's 6540*4 fs = 25
  picoseconds).
  savesteps=6250
else
  # Remove any constraints
  FreeBond all,all
  FreeAngle all,all,all
  # Smaller timestep, since we don't use constraints: 2*1.25 = 2.5 fs
  TimeStep 2,1.25
  ts=2.5
  # Save simulation snapshots every 10000 simulation steps
  # (with a timestep of 2.5 femtoseconds, that's 10000*2.5 fs = 25
  picoseconds).
  savesteps=10000

# Temperature
Temp (temperature)
# Make sure all atoms are free to move
FreeAll
# Alread a snapshot/trajectory present?
i=00000
filename='(MacroTarget)(i).(format)'
running = FileSize (filename)
if not running
  # Perform energy minimization
  Experiment Minimization
  Experiment On
  Wait ExpEnd
  # And now start the real simulation
  Sim On
else
  # Simulation has been running before
  ShowMessage "Simulation has been running before, loading last
  snapshot..."
  Wait 1
  # Switch console off to load the snapshots quickly
  Console Off
if format=='sim'
    # Find and load the last 'sim' snapshot
    do
        i = i+1
        found = FileSize (MacroTarget)(i).sim
    while found
        i=i-1
        LoadSim (MacroTarget)(i)
    else
        # XTC format requires that the entire trajectory is read in to find
        the last one
        do
            i = i+1
            eof,time = LoadXTC (filename),(i)
            ShowMessage 'Searching XTC trajectory for last snapshot, showing
            snapshot (i) at (0+time) fs'
            Sim Pause
            Wait 1
            while !eof
                Sim Continue
            # Adjust savesteps to save snapshots in the same interval as previously
            if i>0
                t = Time
                savesteps=0+t/(ts*i)
                #print 'Time=(t), TimeStep=(ts), savesteps=(savesteps)'
            HideMessage
        # Set temperature and pressure control
        TempCtrl Rescale
        PressureCtrl (pressurectrl)
        # Uncomment to add distance constraints
        # AddSpring O Res Lys 80,H Res Glu 84,Len=1.9
        # And finally, make sure that future snapshots are saved
        Save(format) (filename),(savesteps)
    if duration=='forever'
        Console On
        Wait forever
    else
        Console Off
        # Wait for given number of picoseconds
        do
            Wait 10
            t = Time
        while t<duration*1000
        Sim Off

    # Number of the object whose RMSDs from the starting conformation will be
    calculated
    # If the protein is an oligomer, check the documentation of the 'Sup' command at 'analyzing a simulation' to avoid pitfalls.
currobj = 1

# Forcefield to use (these are all YASARA commands, so no '=' used)
# Use YASARA2 in YASARA Structure to include a quality Z-score
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# The B-factors calculated from the root-mean-square fluctuations can be
# too large to fit them into the PDB file's B-factor column. Replace e.g. 1.0 with 0.1 to scale
# them down to 10%
bfactorscale=1.0

# Flag to save a PDB file of the solute snapshots for further analysis
pdbsaved=0

# Selection of atoms to include for 'Calpha' RMSD calculation (also
# consider DNA/RNA)
casel='CA Protein or C1* NucAcid'

# Selection of atoms for which the dynamic cross-correlation matrix (DCCM)
# should be visualized.
# Here are some typical examples:
# dccmsel='' - Don't calculate the DCCM, the default
# dccmsel='Atom CA Protein' - Calculate the DCCM for protein Calpha atoms
# dccmsel='Res Protein' - Calculate the DCCM for protein residue centers
# dccmsel=''

# Selection of atoms for which the radial distribution function (RDF)
# should be visualized
# Here are some examples:
# rdfsel='' - Don't calculate the DCCM, the default
# rdfsel='O Res HOH,O Res HOH,Bins=40,BinWidth=0.25'
# - Calculate the RDF of water in 40 bins, each 0.25 A wide (thus up to 10 A).
# rdfsel='CG Res Asp 120,ND1 Res His 200,Bins=20,BinWidth=0.5'
# - Calculate the RDF between two specific atoms in 20 bins, each 0.25 A wide
#   (thus again up to 10 A). Note that you may have to save more
#   snapshots than
#   usually in md_run.mcr to avoid problems with sparse data and
#   noisy RDF results.
# rdfsel=''
# First snapshot to be analyzed, increase number to ignore an equilibration period.
# (By default, md_run.mcr saves snapshots every 25ps, choosing 40 thus starts the analysis after 1 nanosecond)
firstsnapshot=0

# No change required below this point
# ==============================================================

# Do we have a target?
if MacroTarget==''
    RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to choose a target structure"
Clear
Console Off
# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
    RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water

calphas = CountAtom (casel)
if calphas>0 and calphas<3
    # We cannot superpose 1 or 2 Calpha atoms
    casel='None'

ShowMessage "Preparing analysis, please wait..."
Wait 1

# See if structure validation checks should be done (require YASARA2 force field)
checked=0
fof = ForceField
if fof=='YASARA2'
    checked=1

# Duplicate the intial object for RMSD calculation
startobj = DuplicateObj (currobj)
RemoveObj (startobj)

i=00000+firstsnapshot
emin=1e99
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    # Add time in picoseconds to table
simtime = Time
ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
Wait 1
Tabulate (simtime/1000)
  # Get energy components, including packing energies for YASARA2 force field
  if checked
  
ebndlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i),pa
cking1,packing3 = EnergyAll All
  else
  
ebndlist(i),eanglist(i),edihlist(i),eplnlist(i),ecoulist(i),evdwlist(i) = EnergyAll All
      packing1=0
      packing3=0
  elist(i) = ebndlist(i)+eanglist(i)+edihlist(i)+eplnlist(i)+ecoulist(i)+evdwlist(i)+pa
cking1+packing3
  # The following examples provide a few hints for other things to analyze.
  # If you uncomment one of the examples, keep in mind that every value you
  # tabulate becomes an additional column in the table, so you must increase the
  # 'Columns' parameter of the SaveTab command further below (and the table
  # header will also no longer indicate the proper results unless you adapt it).
  
  # Example: Measure the distance between the carboxyl group of Glu 123 (Cdelta)
  # and the guanidinium group of Arg 345 (Czeta):
  # Tabulate Distance CD Res Glu 123, CZ Res Arg 345
  
  # Example: Measure the distance between two centers of mass, e.g. the loop from
  # residue Ala 205 to Glu 210, and the ligand NAD:
  # cenA() = GroupCenter Res Ala 205 - Glu 210, Type=Mass
  # cenB() = GroupCenter Res NAD, Type=Mass
  # Tabulate (norm (cenA-cenB))
  
  # Example: Check if the carboxyl group of Glu 123 and the guanidinium group of
  # Arg 345 are currently hydrogen-bonded (1) or not (0):
  # hbolist() = ListHBoAtom Sidechain Res Glu 123, Sidechain Res Arg 345
  # Tabulate (count hbolist>0)
  
  # Example: Count the number of atoms in molecule A that are hydrogen bonded to B
  # hbolist() = ListHBoAtom Mol A,Mol B
  # Tabulate (count hbolist)
  
  # Example: Calculate the current potential energy of residue Glu 123:
# Tabulate EnergyRes Glu 123
#
# Example: Calculate the backbone RMSD for residues 1-120:
# Tabulate SupAtom Backbone Res 1-120 Obj (currobj),Backbone Res 1-120 Obj (startobj)
#
# Save the minimum energy structure (ignoring solvent-solvent interactions)
e = EnergyObj (currobj)
if checked
    # Calculate structure validation Z-scores, using the formula from homology modeling
    for type in 'dihedrals','packing1d','packing3d'
        zscore(type) = CheckObj (currobj),(type)
    zscorelist(i) = zscoredihedrals*0.145+zscorepacking1d*0.390+zscorepacking3d*0.465
if rdfsel=''
    # Collect data for radial distribution function
    BinDistance (rdfsel)
    Sim Off
if e<emin
    emin=e
SaveSce (MacroTarget)_energymin
if pdbsaved
    # Save a PDB file of the solute
    SavePDB (currobj),(MacroTarget)_(i)
    # Add CA, backbone and heavy atom RMSDs to table
    AddObj (startobj)
    # Trick: If the solute object contains neither CA nor backbone atoms,
    # we simply assign the SupAtom error code (=0)
    carmsdlist(i) = SupAtom (casel) and Obj (currobj),(casel) and Obj (startobj)
    bbrmsdlist(i) = SupAtom Backbone Obj (currobj),Backbone Obj (startobj)
    aarmsdlist(i) = SupAtom Element !H Obj (currobj),Element !H Obj (startobj)
    # Add results to table
    Tabulate (elist(i)),(ebndlist(i)),(eanglist(i)),(edihlist(i)),(eplnlist(i)),(ecoulist(i)),(evdwlist(i)),
        (carmsdlist(i)),(bbrmsdlist(i)),(aarmsdlist(i))
    if checked
        Tabulate (zscorelist(i))
    # Add the current atom positions to internal table to obtain RMSF and average positions
    AddPosAtom Obj (currobj)
    RemoveObj (startobj)
    # Next snapshot
    i=i+1
if !i
    RaiseError "This macro is meant to analyze a molecular dynamics trajectory created with md_run, but none was found in this directory"
# Add average results to table
Tabulate 'Average',(mean elist),(mean ebndlist),(mean eanglist),(mean edihlist),
(mean eplnlist), (mean ecoulist), (mean evdwlist), (mean carmsdlist), (mean
bbrmsdlist), (mean aarmsdlist)
header='____Time[ps] Energy[(EnergyUnit)]_______Bond _______Angle
____Dihedral ___Planarity_______Coulomb _________VdW _RMSDs[A]:CA
____Backbone __HeavyAtoms'
if checked
    header=header+' QualityScore'
Tabulate (mean zscorelist)
# Save main analysis table
SaveTab
default,(MacroTarget)_analysis,Format=Text,Columns=(11+checked),NumFormat=
12.3f,(header)

# Calculate time-average structure and set B-factors according to RMSF
AveragePosAtom Obj (currobj)
RMSFAtom Obj (currobj),Unit=BFactor
if bfactorscale!=1.0
    # Scale B-factors so that they fit into the PDB format
    first,last=SpanAtom Obj (currobj)
    for i=first to last
        bf=BFactorAtom (i)
        BFactorAtom (i),(bf*bfactorscale)
    # The time average structure has incorrect covalent geometry and should be
    energy minimized
    SavePDB (currobj),(MacroTarget)_average

""
# Example: Create an additional RMSF file, in case B-factors are too large
for the PDB format
DelTab default
first,last = SpanAtom Obj (currobj)
rmsflist() = RMSFAtom Obj (currobj)
for i=first to last
    res = ListAtom (i),Format='RESNAME,RESNUM'
    Tabulate (i),(res),(rmsflist(i-first+1))
SaveTab
default,(MacroTarget)_rmsf,Format=Text,Columns=4,NumFormat=8.2f,"RMSF
Table"
""
if rdfsel!=''
    # Additionally calculate and show the radial distribution function
    (RDF).
    MakeTab RDF,Dimensions=1
    Tabulate RDF
    SaveTab RDF,(MacroTarget)_rdf,Format=Text,Columns=1,NumFormat=6.3f,
    'Radial distribution function with parameters (rdfsel)'
    obj = ShowTab RDF,Width=1.0,Range=10,MinCol=Blue,MaxCol=Yellow
    PosObj (obj),X=0,Y=-12,Z=31
    RotateObj (obj),X=-90
    SaveSce (MacroTarget)_rdf
DelObj (obj)

if dccmsel!=''
    # Additionally calculate and show the dynamic cross-correlation matrix (DCCM).
    # This matrix correlates the displacements from the time average structure,
    # see the documentation of the 'DCCM' command for details.
    # First get the number of selected units, i.e. the rows/columns in the matrix
    units = Count(dccmsel)
    if !units
        RaiseError 'The DCCM selection (dccmsel) did not match any atoms'
    # Take the time average structure as the start object to superpose onto
    DelObj (startobj)
    startobj = DuplicateObj (currobj)
    RemoveObj (startobj)
    # Loop over the snapshots a second time to calculate the displacements from the time average
    i=00000+firstsnapshot
    while 1
        # See if next snapshot is present
        sim = FileSize (MacroTarget)(i).sim
        if not sim
            break
        # Yes, load it
        LoadSim (MacroTarget)(i)
        Sim Pause
        ShowMessage 'Calculating dynamic cross-correlation matrix, analyzing snapshot (0+i)...'
        Wait 1
        Sim Off
        # Superpose snapshot on the time average structure
        AddObj (startobj)
        SupAtom (casel) and Obj (currobj),(casel) and Obj (startobj)
        # Add the current displacements to an internal table to obtain the DCCM
        AddDisp(dccmsel) Obj (currobj),(dccmsel) Obj (startobj)
        RemoveObj (startobj)
        # Next snapshot
        i=i+1
    # Store the DCCM in a table
    MakeTab DCCM,Dimensions=2,Columns=(units)
    Tabulate DCCM
    # Visualize the DCCM
    pointwidth=1.
    height=5.
    dccmobj1 = ShowTab DCCM,Width=(pointwidth),Range=(height),Min=-1,Max=1.0
    # By default, ShowTab shows the minimum at Z=0, move so that correlation 0 is at Z=0
    MoveObj (dccmobj1),Z=(height*0.5)
    # Visualize the zero level with a flat DCCM wireframe
    dccmobj2 = ShowTab DCCM,Width=(pointwidth),Range=0,Min=-1,Max=1.0
    dccmobj3 = ShowWireObj (dccmobj2),Static,Mesh=Solid
DelObj (dccmobj2)
PointPar Radius=0.5, Plastic=No
NameObj (dccmobj3), ZeroLevel
RotateObj (dccmobj1) (dccmobj3), X=180

# Create a text object with the residue names and the table header
textwidth = pointwidth * units * 2

# Duplicate the labels at the bottom

# Forcefield to use (these are all YASARA commands, so no '=' used)
ForceField AMBER03

# Cutoff
Cutoff 7.86

# Cell boundary
Boundary periodic

# Use longrange coulomb forces (particle-mesh Ewald)
Longrange Coulomb

# Consider protein residues with a Calpha plus nucleic acid residues with a C1*
atomsel = 'Atom CA Protein or Atom C1* NucAcid'

# First snapshot to be analyzed, increase number to ignore an equilibration period.
# (By default, md_run.mcr saves snapshots every 25ps, choosing 40 thus starts the analysis after 1 nanosecond)
firstsnapshot = 0

# No change required below this point
# ______________________________

# Do we have a target?
if MacroTarget == ''
RaiseError "This macro requires a target. Either edit the macro file or click Options > Macro > Set target to choose a target structure"

Clear
Console Off
# Do we have a scene with water?
scene = FileSize (MacroTarget)_water.sce
if not scene
    RaiseError 'Could not find initial scene file (MacroTarget)_water.sce'

# Load the scene
LoadSce (MacroTarget)_water

# We need at least 3 Calpha atoms to superpose
calphas = CountAtom (atomsel)
if calphas<3
    RaiseError 'This macro currently requires at least three residues to analyze, because it performs a superposition and RMSD calculation'

ShowMessage "Preparing analysis, please wait..."
Wait 1

# Duplicate the intial object for RMSD calculation
startobj = DuplicateObj (currobj)

# Get a selection of residues that match atomsel in the current and the start objects
for type in 'curr','start'
    reslist() = ListRes (atomsel) and Obj ((type)obj)
    (type)ressel=join reslist
RemoveObj (startobj)

# Set the summed up RMSDs for CA, Backbone and HeavyAtoms to zero
rmsds=count reslist
for i=1 to 3
    for j=1 to rmsds
        rmsd(i)sum(j)=0.

i=00000+firstsnapshot
while 1
    # See if next snapshot is present
    sim = FileSize (MacroTarget)(i).sim
    if not sim
        break
    # Yes, load it
    LoadSim (MacroTarget)(i)
    Sim Pause
    simtime = Time
    ShowMessage 'Analyzing snapshot (0+i) at (0+(simtime/1000)) ps'
    Wait 1
    # Get per residue RMSDs between current residue selection and start residue selection
    AddObj (startobj)
rmsd1() = SupAtom (atomsel) and Obj (currobj), (atomsel) and Obj (startobj), Unit=Res
rmsd2() = SupAtom Res (currressel) Backbone, Res (startressel) Backbone, Unit=Res

# Sum up atom positions to calculate RMSFs
AddPosAtom Res (currressel)
# Sum up RMSDs
for j=1 to 3
  for k=1 to rmsds
    rmsd(j)sum(k)=rmsd(j)sum(k)+rmsd(j)(k)
  RemoveObj (startobj)
# Next snapshot
i=i+1

if !i
  RaiseError "This macro is meant to analyze a molecular dynamics trajectory created with md_run, but none was found in this directory"
# Calculate the average
rmsflist() = RMSFRes (atomsel) and Obj (currobj)
reslist() = ListRes (atomsel) and Obj (currobj), Format='RESNAME RESNUM MOLNAME'
for j=1 to rmsds
  Tabulate '(reslist(j))', (rmsd(1)sum(j)/i), (rmsd(2)sum(j)/i), (rmsd(3)sum(j)/i), (rmsf list(j))
# Save table
SaveTab default, (MacroTarget)_analysisres, Format=Text, Columns=5, NumFormat=%12.3f, _ _ _Residue _RMSDs[A]:CA ____Backbone __HeavyAtoms______RMSF[A]
HideMessage

Exit