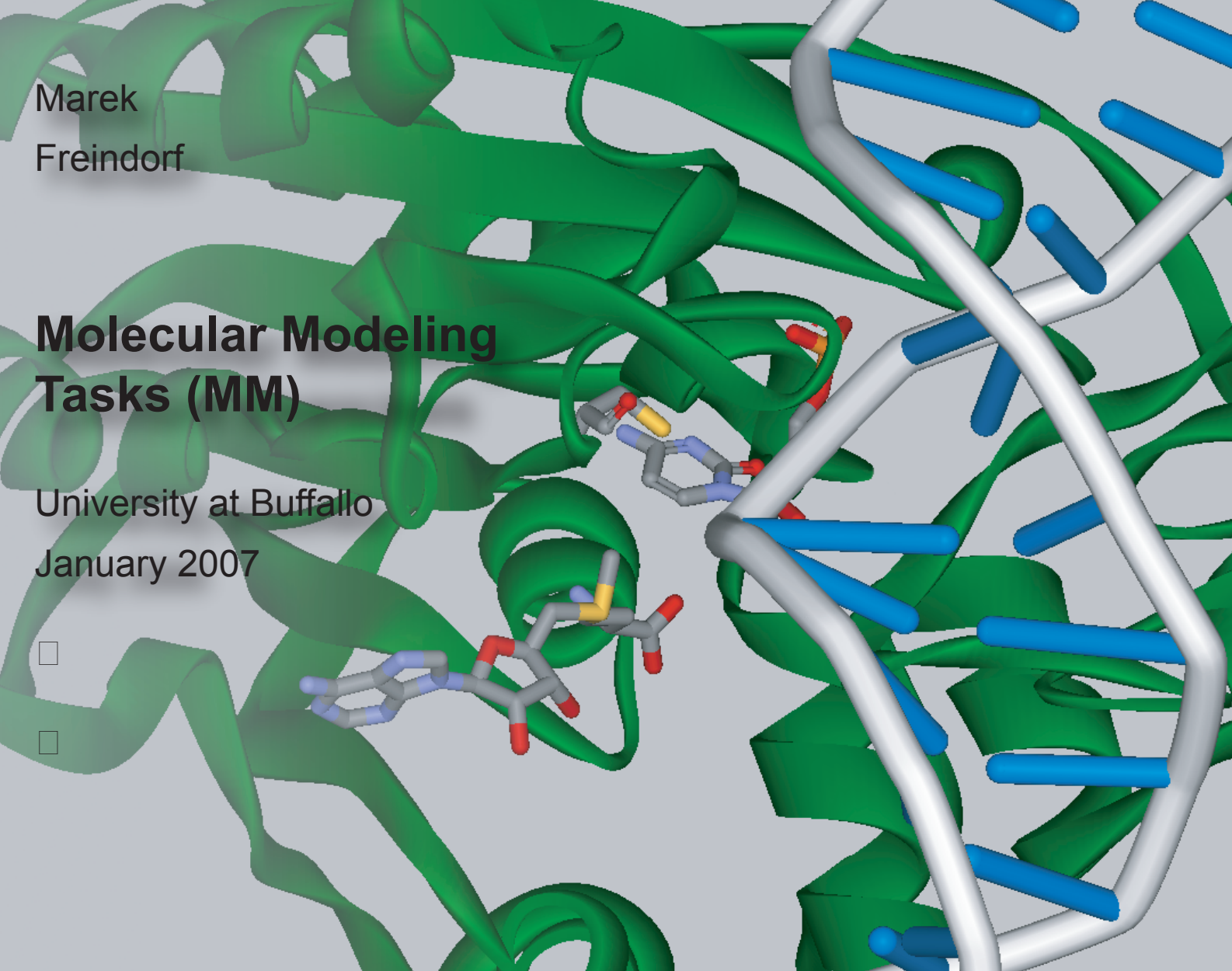
Marek
Freindorf

# Molecular Modeling Tasks (MM)

University at Buffallo

January 2007

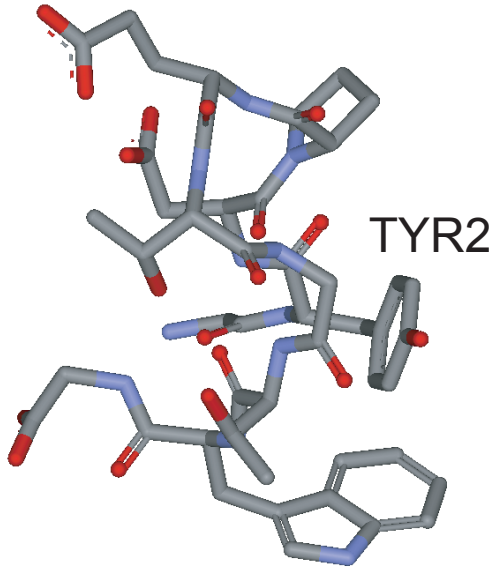


# MM minimization of small proteins (MM-1)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field

2. Replace manually tyrosine TYR2 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

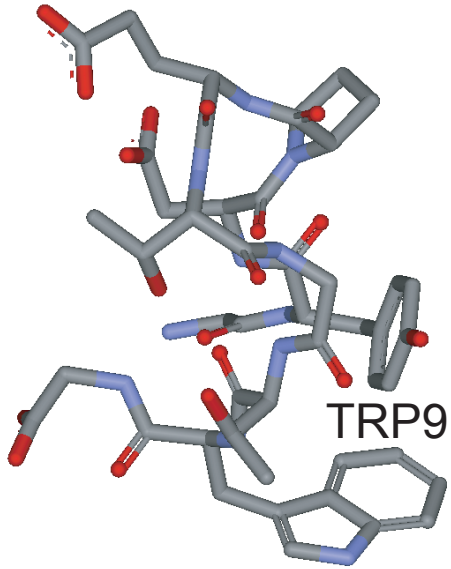
5. Report results of the same calculations for the TYR2 -> VAL, TYR2 -> SER, and TYR2 -> THR mutations

# MM minimization of small proteins (MM-2)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field

2. Replace manually tryptophan TRP9 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein

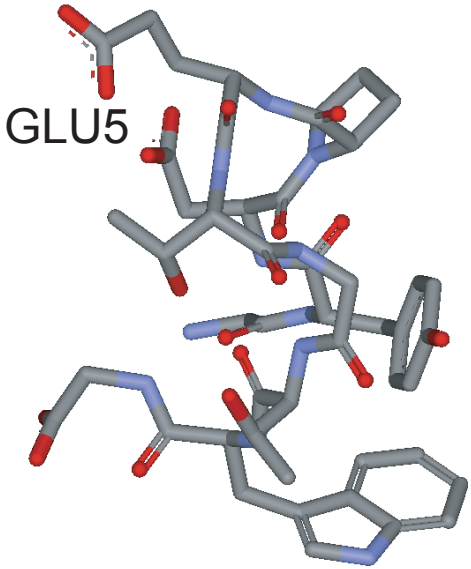



4. Report in a figure the total energy of the protein as a function of minimization steps

5. Report results of the same calculations for the TRP9 -> VAL, TRP9 -> SER, and TRP9 -> THR mutations

# MM minimization of small proteins (MM-3)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field




2. Replace manually glutamic acid GLU5 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein

4. Report in a figure the total energy of the protein as a function of minimization steps

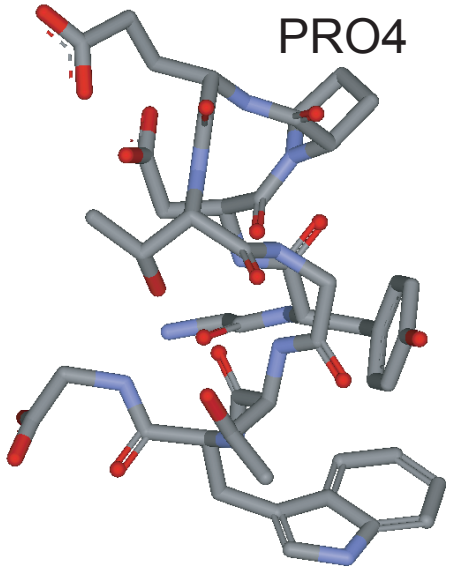
5. Report results of the same calculations for the GLU5 -> VAL, GLU5 -> SER, and GLU5 -> THR mutations

# MM minimization of small proteins (MM-4)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field

2. Replace manually proline PRO4 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

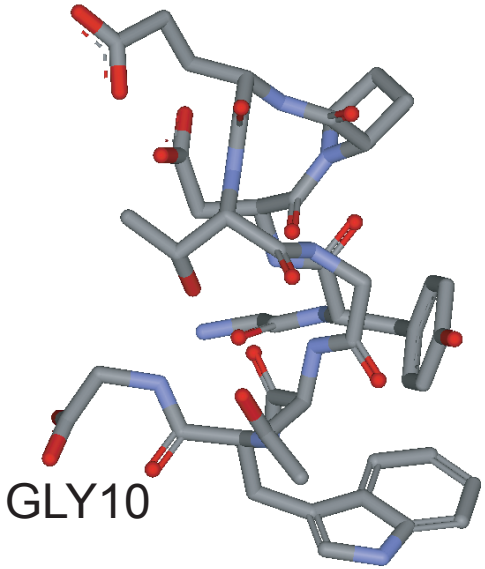
5. Report results of the same calculations for the PRO4 -> VAL, PRO4 -> SER, and PRO4 -> THR mutations

# MM minimization of small proteins (MM-5)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field

2. Replace manually glycine GLY10 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

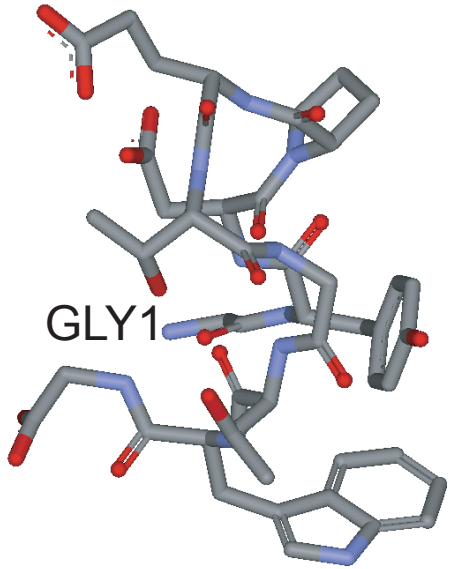
5. Report results of the same calculations for the GLY10 -> VAL, GLY10 -> SER, and GLY10 -> PRO mutations

# MM minimization of small proteins (MM-6)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field

2. Replace manually glycine GLY1 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein

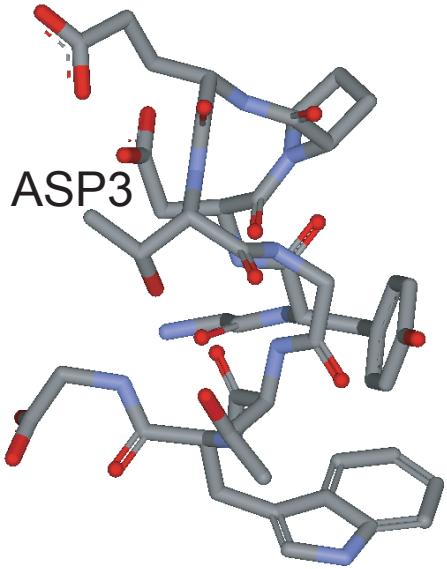



4. Report in a figure the total energy of the protein as a function of minimization steps

5. Report results of the same calculations for the GLY1 -> VAL, GLY1 -> SER, and GLY1 -> PRO mutations

# MM minimization of small proteins (MM-7)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field




2. Replace manually aspartic acid ASP3 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein

4. Report in a figure the total energy of the protein as a function of minimization steps

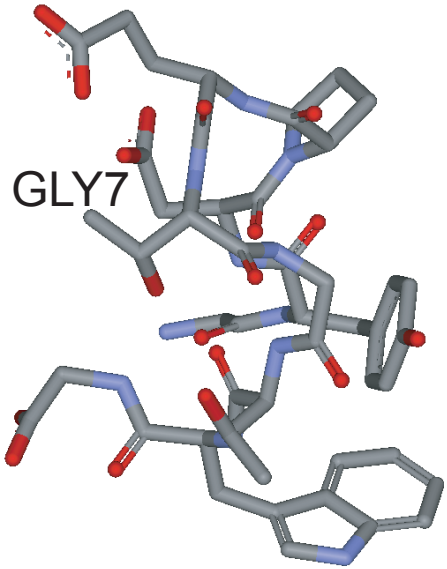
5. Report results of the same calculations for the ASP3 -> VAL, ASP3 -> SER, and ASP3 -> PRO mutations

# MM minimization of small proteins (MM-8)

1. Calculate an energy minimization of Chignolin, starting from the initial PDB file, using AMBER force field

2. Replace manually glycine GLY7 by lysine in the initial PDB file

3. Repeat an energy minimization of the mutated protein

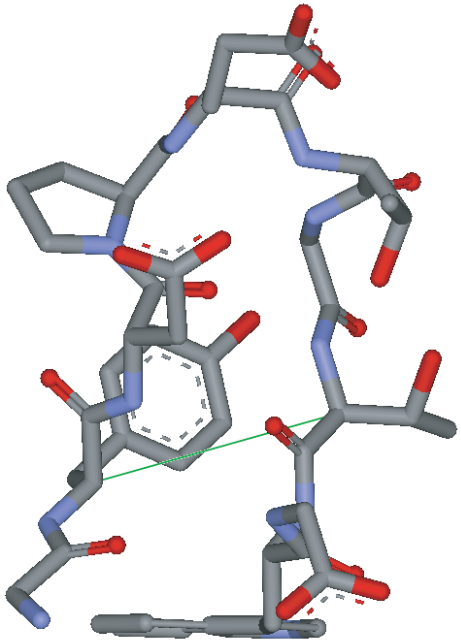



4. Report in a figure the total energy of the protein as a function of minimization steps

5. Report results of the same calculations for the GLY7 -> VAL, GLY7 -> SER, and GLY7 -> PRO mutations

# MM constrained minimization of small proteins (MM-9)

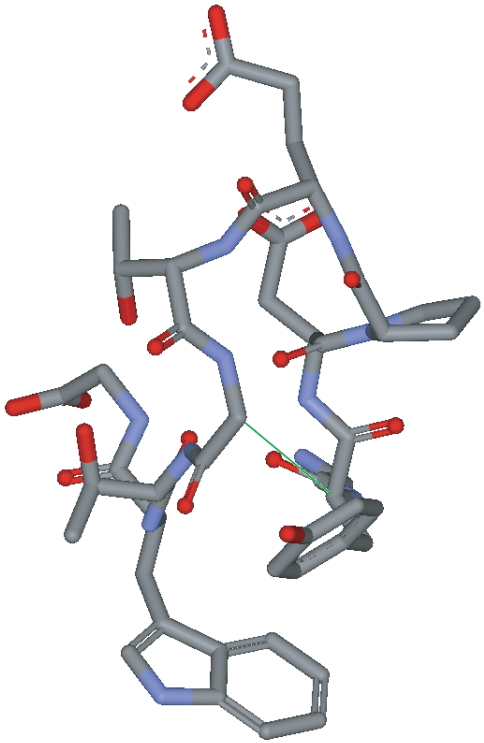
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 8A, between CA atom of TYR2 and CA atom of THR8
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 10A, between those two atoms

# MM constrained minimization of small proteins (MM-10)

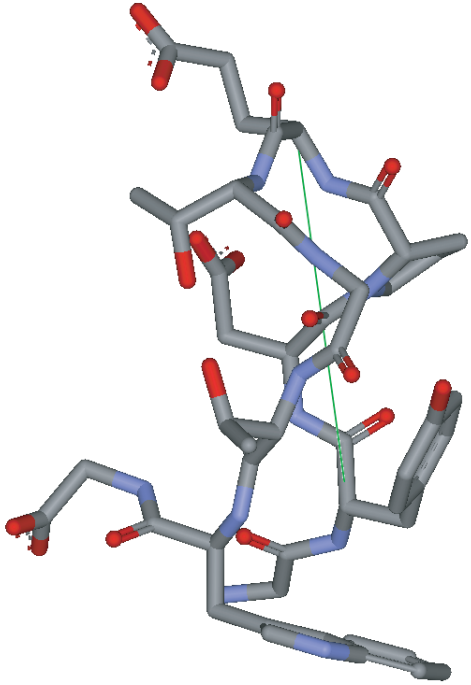
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of TYR2 and CA atom of GLY7
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 12A, between those two atoms

# MM constrained minimization of small proteins (MM-11)

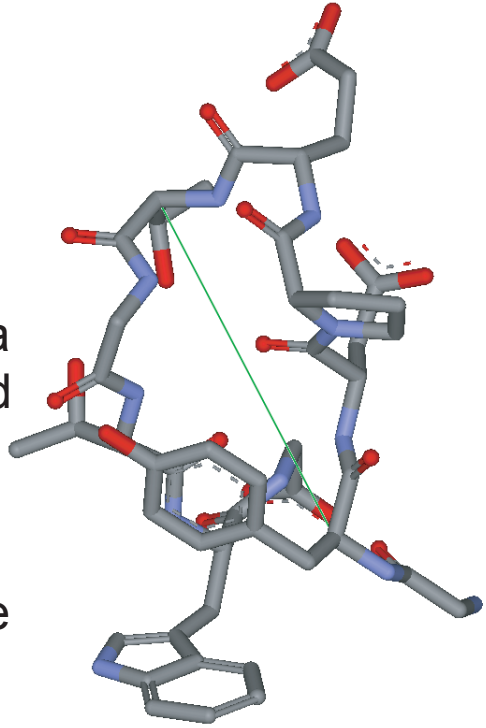
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of TYR2 and CA atom of GLU5
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 12A, between those two atoms

# MM constrained minimization of small proteins (MM-12)

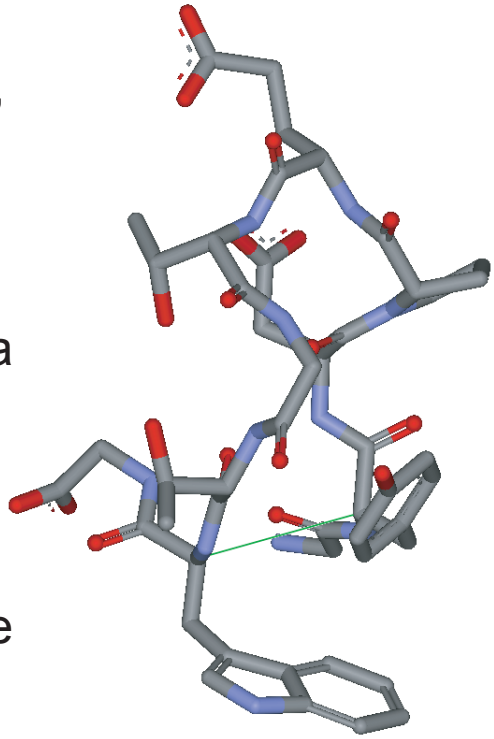
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of TYR2 and CA atom of THR6
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 12A, between those two atoms

# MM constrained minimization of small proteins (MM-13)

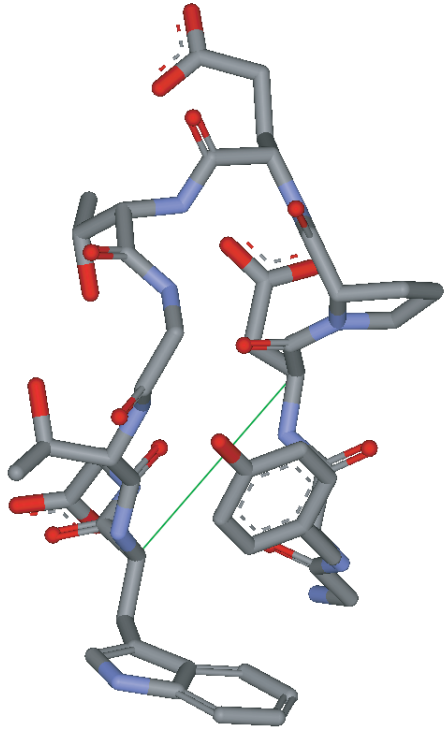
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 6A, between CA atom of TYR2 and CA atom of TRP9
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 10A, between those two atoms

# MM constrained minimization of small proteins (MM-14)

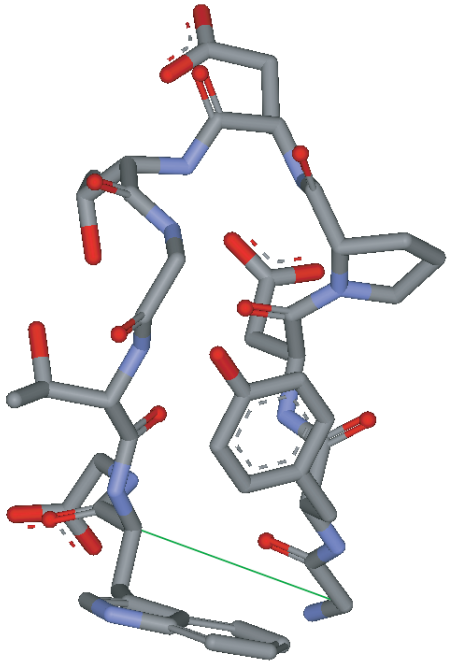
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 7A, between CA atom of TRP9 and CA atom of ASP3
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 12A, between those two atoms

# MM constrained minimization of small proteins (MM-15)

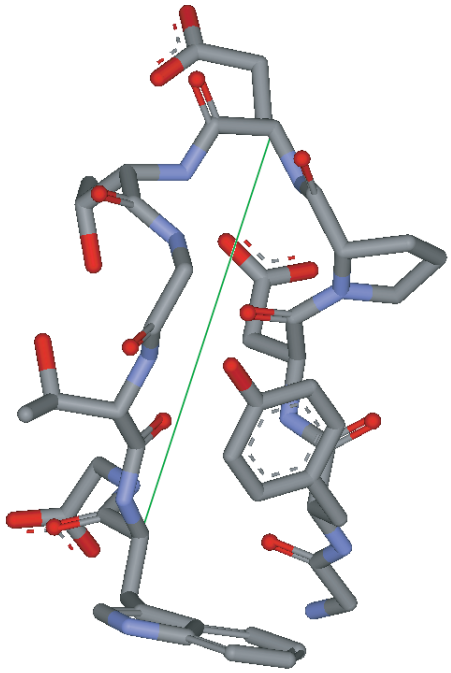
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 7A, between CA atom of TRP9 and CA atom of GLY1
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 12A, between those two atoms

# MM constrained minimization of small proteins (MM-16)

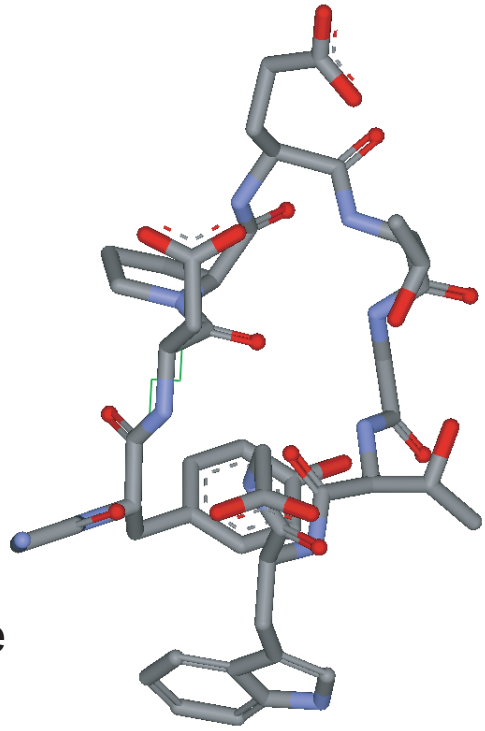
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 8A, between CA atom of TRP9 and CA atom of GLU5
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 15A, between those two atoms

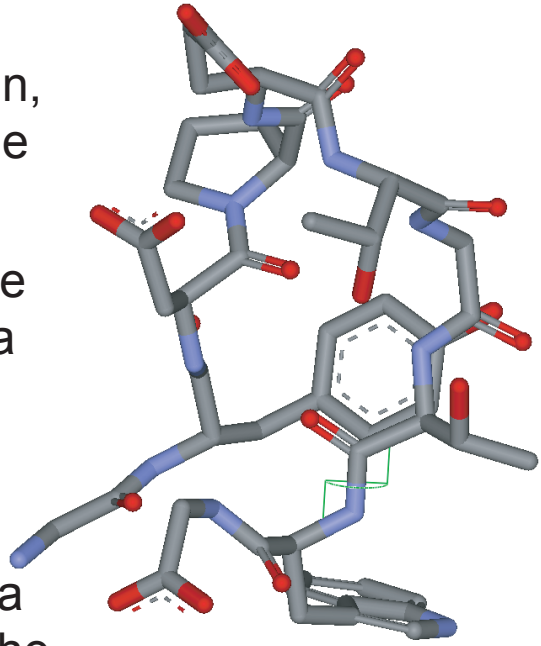
# MM constrained minimization of small proteins (MM-17)

1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between C and N atoms of TYR2, and CA and C atoms of ASP3
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM constrained minimization of small proteins (MM-18)

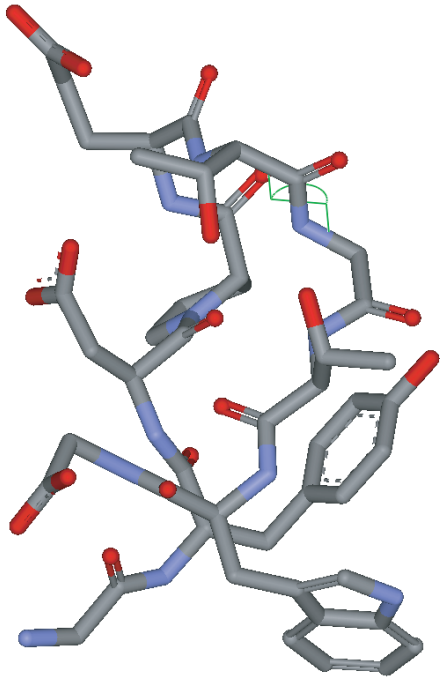


1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between CA and C atoms of THR8, and N and CA atoms of TRP9
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints

5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM constrained minimization of small proteins (MM-19)

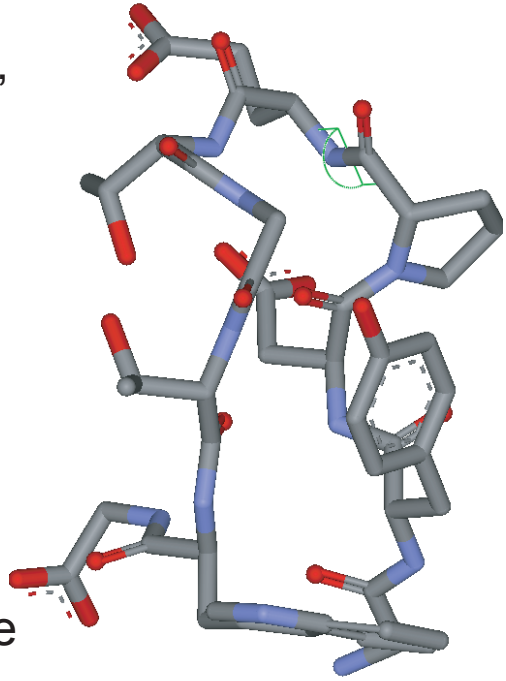
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between CA and C atoms of THR6, and N and CA atoms of GLY7
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM constrained minimization of small proteins (MM-20)

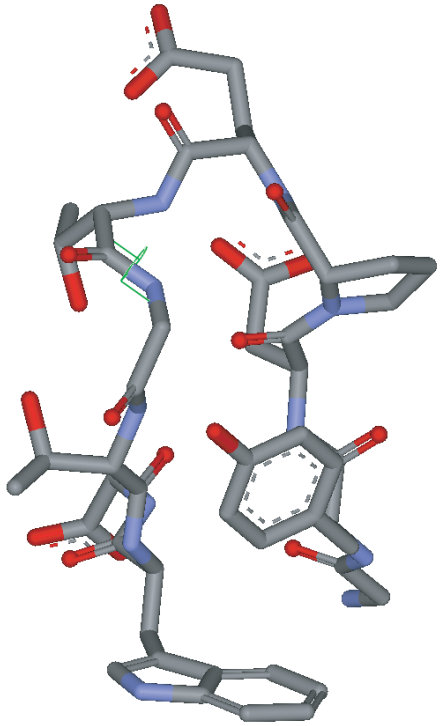
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between CA and N atoms of GLU5, and C and CA atoms of PRO4
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM constrained minimization of small proteins (MM-21)

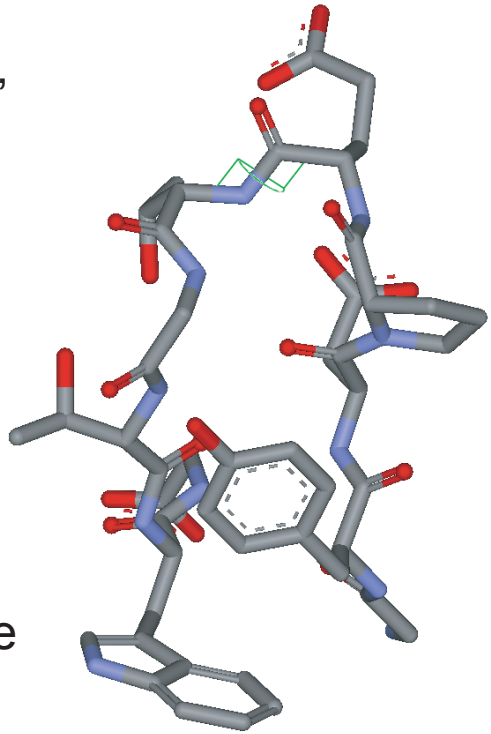
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between CA and C atoms of THR6, and N and CA atoms of GLY7
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM constrained minimization of small proteins (MM-22)

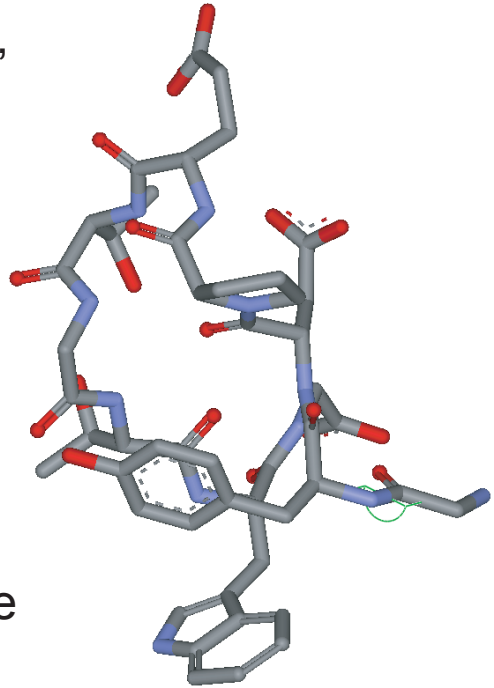
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between CA and C atoms of GLU5, and N and CA atoms of THR6
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM constrained minimization of small proteins (MM-23)

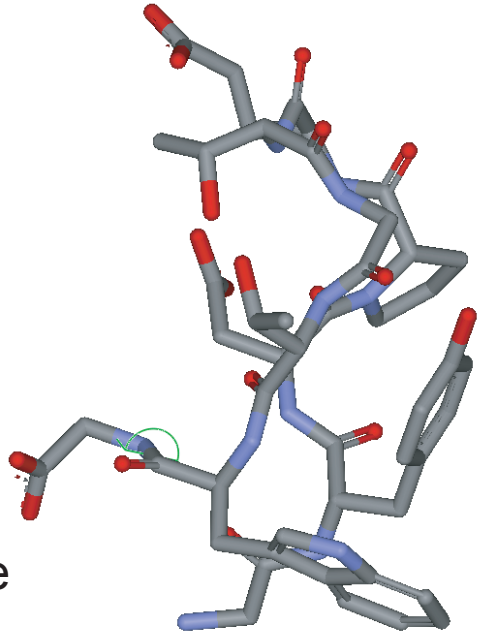
1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between CA and C atoms of GLY1, and C and N atoms of TYR2
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM constrained minimization of small proteins (MM-24)

1. Perform energy minimization of Chignolin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a torsion constraint of a value 180 degrees, between CA and C atoms of TRP9, and N and CA atoms of GLY10
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



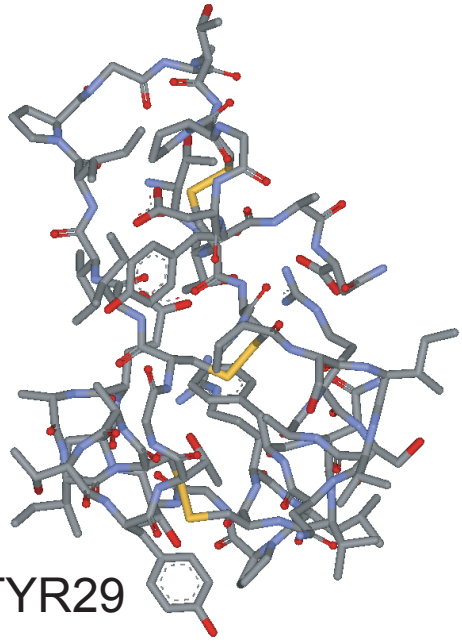
5. Repeat the similar energy minimization and report results of the calculations for the constraint value 0 degrees, between those four atoms

# MM minimization of medium proteins (MM-25)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually TYR29 by PRO in the initial PDB file

3. Repeat an energy minimization of the mutated protein



TYR29

4. Report in a figure the total energy of the protein as a function of minimization steps

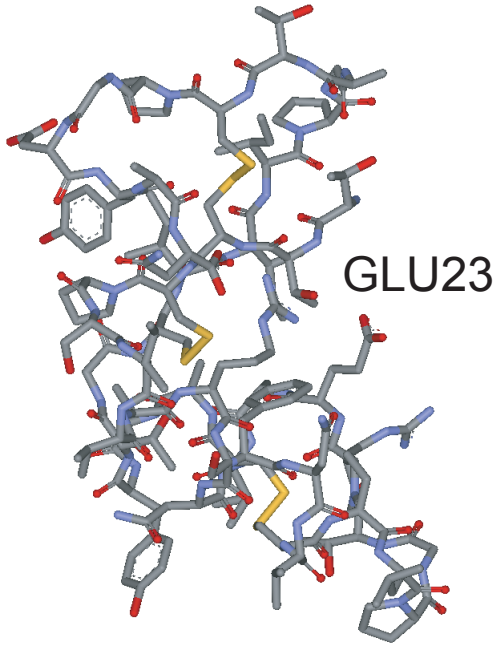
5. Report results of the same calculations for the TYR29 -> VAL, TYR29 -> SER, and TYR29 -> ALA mutations

# MM minimization of medium proteins (MM-26)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually GLU23 by LYS in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

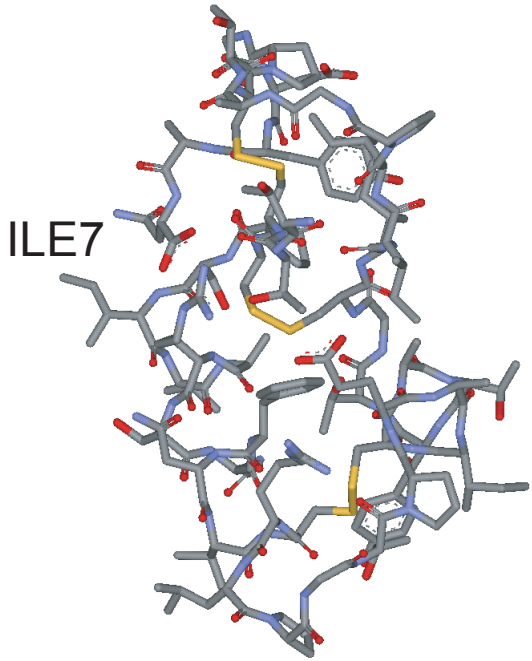
5. Report results of the same calculations for the GLU23 -> VAL, GLU23 -> SER, and GLU23 -> THR mutations

# MM minimization of medium proteins (MM-27)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually ILE7 by LYS in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

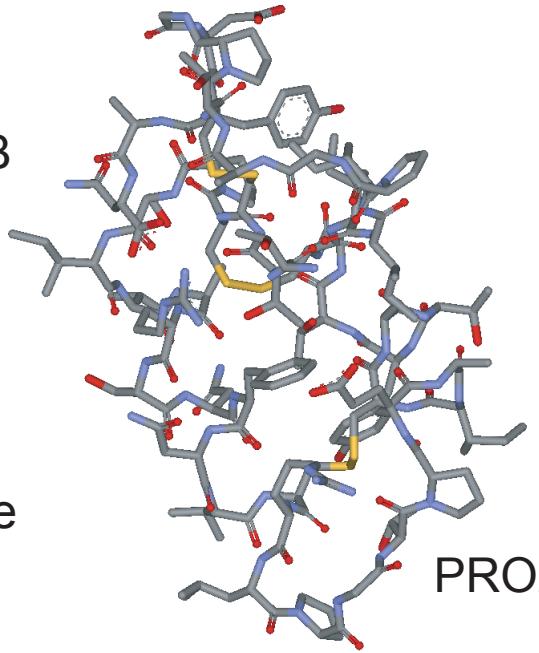
5. Report results of the same calculations for the ILE7 -> VAL, ILE7 -> SER, and ILE7 -> THR mutations

# MM minimization of medium proteins (MM-28)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually PRO22 by LYS in the initial PDB file

3. Repeat an energy minimization of the mutated protein



PRO22

4. Report in a figure the total energy of the protein as a function of minimization steps

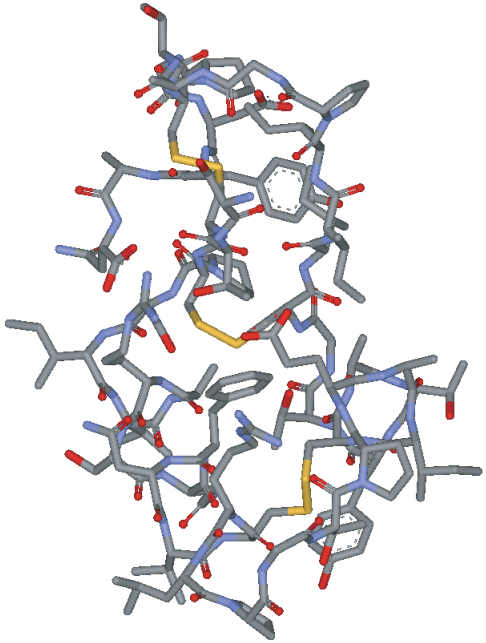
5. Report results of the same calculations for the PRO22 -> VAL, PRO22 -> SER, and PRO22 -> THR mutations

# MM minimization of medium proteins (MM-29)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually ALA45 by LYS in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

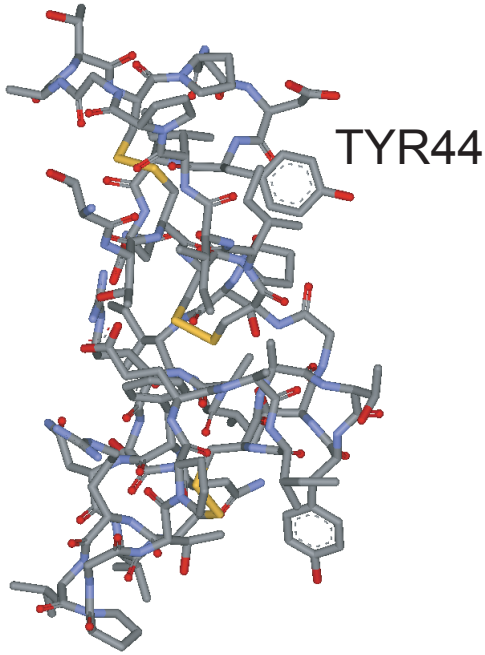
5. Report results of the same calculations for the ALA45 -> VAL, ALA45 -> SER, and ALA45 -> PRO mutations

# MM minimization of medium proteins (MM-30)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually TYR44 by LYS in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

5. Report results of the same calculations for the TYR44 -> VAL, TYR44 -> SER, and TYR44 -> PRO mutations

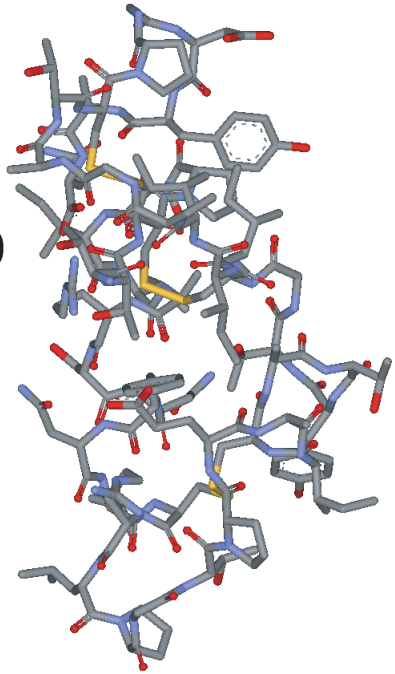
# MM minimization of medium proteins (MM-31)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually ARG10 by LYS in the initial PDB file

3. Repeat an energy minimization of the mutated protein

ARG10



4. Report in a figure the total energy of the protein as a function of minimization steps

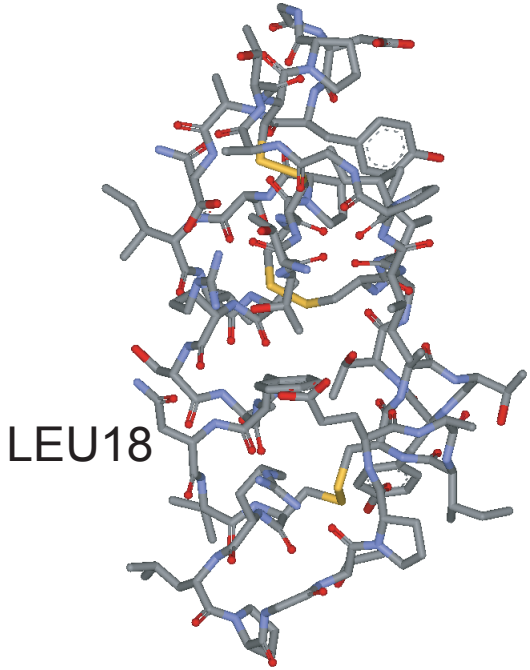
5. Report results of the same calculations for the ARG10 -> VAL, ARG10 -> SER, and ARG10 -> PRO mutations

# MM minimization of medium proteins (MM-32)

1. Calculate an energy minimization of Crambin, starting from the initial PDB file with sulfur bridges

2. Replace manually LEU18 by LYS in the initial PDB file

3. Repeat an energy minimization of the mutated protein




4. Report in a figure the total energy of the protein as a function of minimization steps

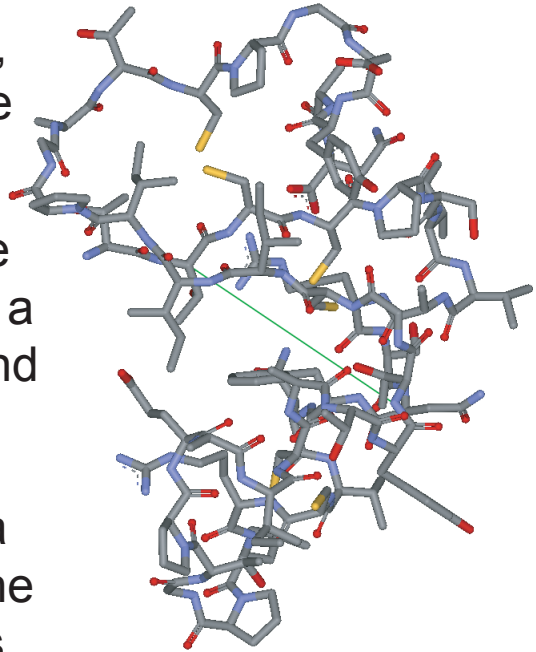
5. Report results of the same calculations for the LEU18 -> VAL, LEU18 -> SER, and LEU18 -> PRO mutations

# MM constrained minimization of medium proteins (MM-33)

1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field

2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of THR2 and CA atom of ASN12

3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



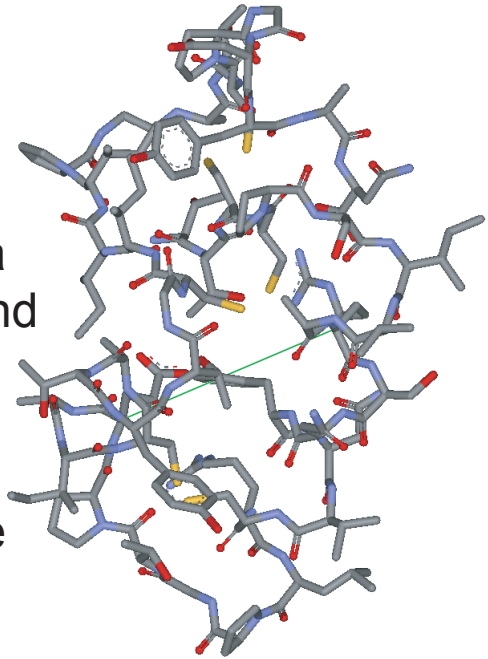
5. Repeat the similar energy minimization and report results of the calculations for the constraint value 16A, between those two atoms

# MM constrained minimization of medium proteins (MM-34)

1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field

2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of GLU23 and CA atom of ARG10

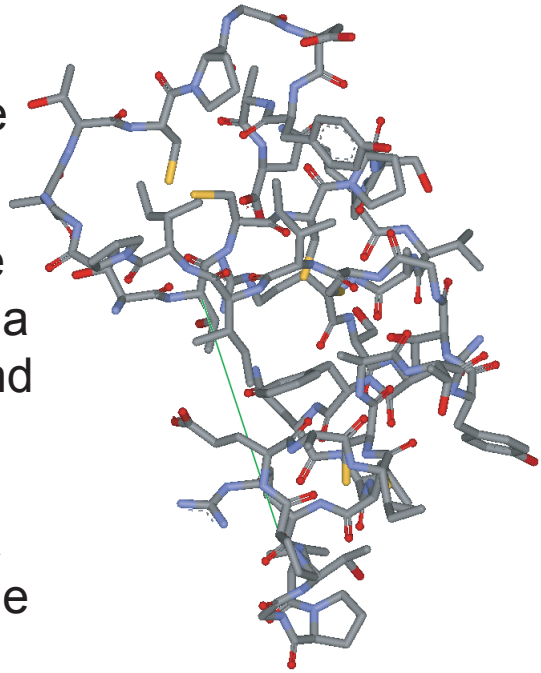
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 16A, between those two atoms

# MM constrained minimization of medium proteins (MM-35)

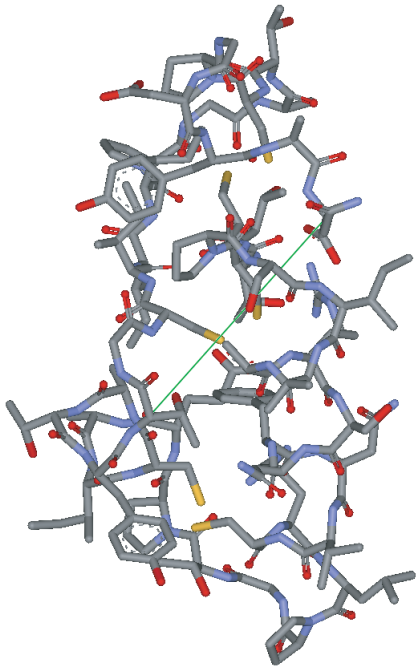
1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of THR2 and CA atom of PRO22
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 16A, between those two atoms

# MM constrained minimization of medium proteins (MM-36)

1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of TYR29 and CA atom of ASN46
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



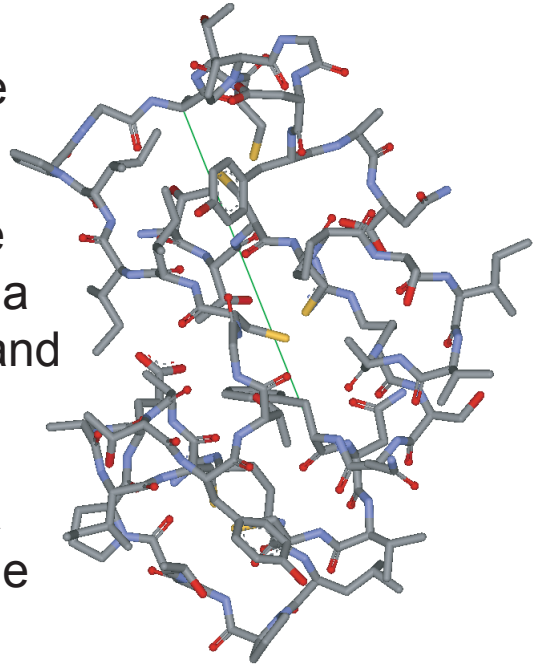
5. Repeat the similar energy minimization and report results of the calculations for the constraint value 16A, between those two atoms

# MM constrained minimization of medium proteins (MM-37)

1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field

2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of PHE13 and CA atom of ALA38

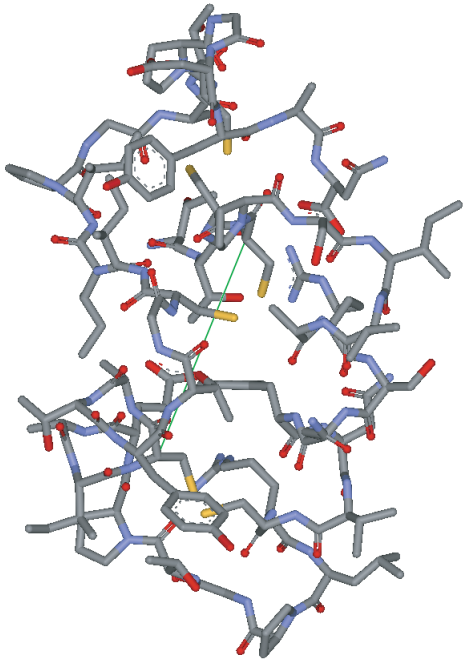
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 16A, between those two atoms

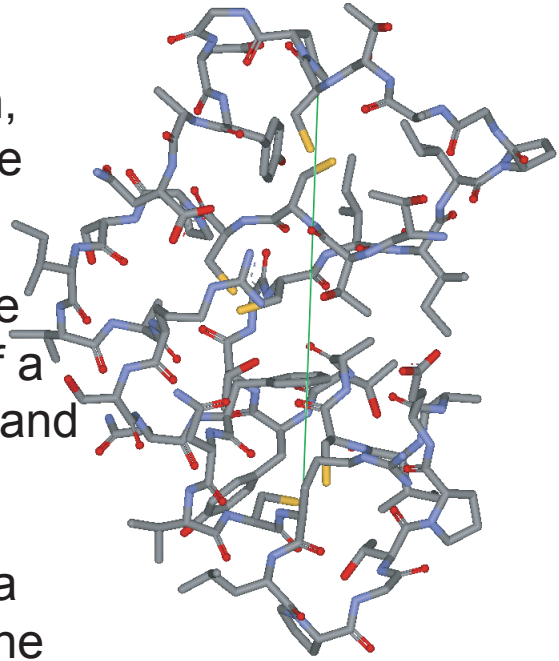
# MM constrained minimization of medium proteins (MM-38)

1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field
2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of CYS4 and CA atom of CYS26
3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 16A, between those two atoms

# MM constrained minimization of medium proteins (MM-39)



1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field

2. Repeat energy minimization for the same protein, applying a distance constraint of a value 20A, between CA atom of ARG17 and CA atom of CYS40

3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints

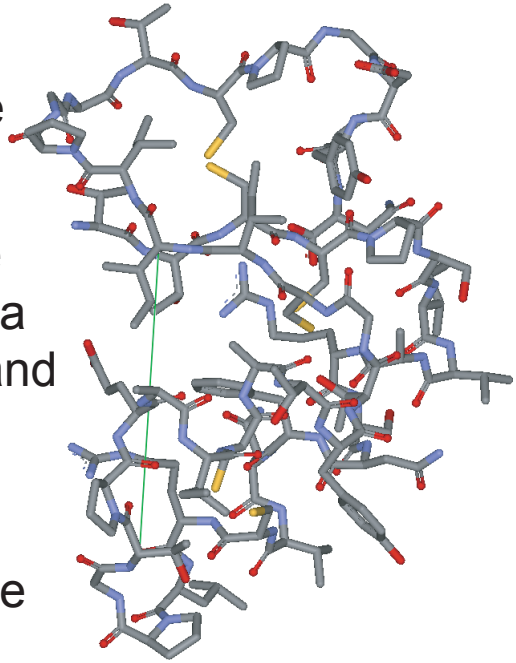
5. Repeat the similar energy minimization and report results of the calculations for the constraint value 14A, between those two atoms

# MM constrained minimization of medium proteins (MM-40)

1. Perform energy minimization of Crambin, starting from the initial PDB file, using the AMBER force field

2. Repeat energy minimization for the same protein, applying a distance constraint of a value 10A, between CA atom of THR21 and CA atom of ILE34

3. Report in a figure the protein energy as a function of minimization steps for both, the minimization with and without constraints



5. Repeat the similar energy minimization and report results of the calculations for the constraint value 14A, between those two atoms

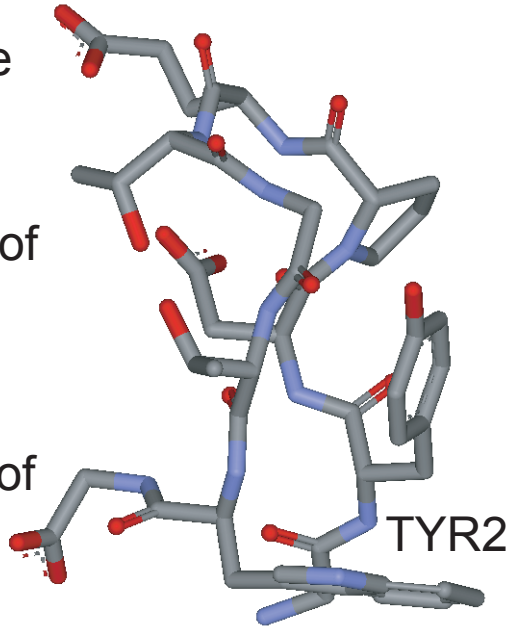
# MM dynamics of small proteins (MM-41)

1. Perform energy minimization of Chignolin, starting from the the TYR2 to TRP protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time




5. Repeat the similar simulations and report results for the TYR2 to ALA protein mutation

# MM dynamics of small proteins (MM-42)

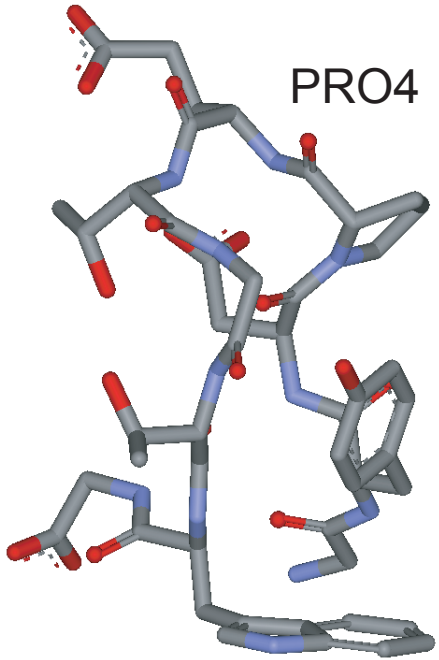
1. Perform energy minimization of Chignolin, starting from the the PRO4 to GLU protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the PRO4 to CYS protein mutation



# MM dynamics of small proteins (MM-43)

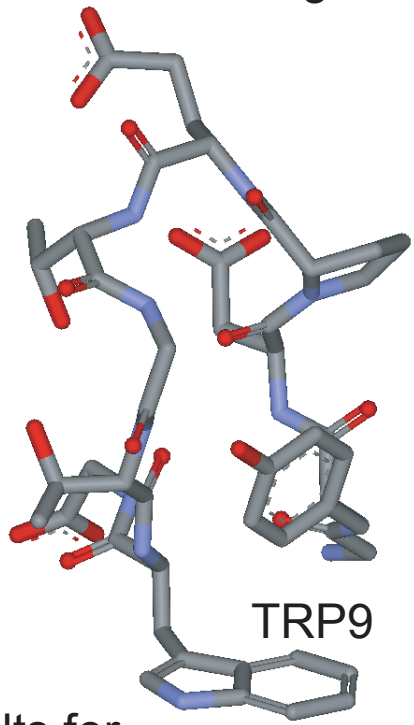
1. Perform energy minimization of Chignolin, starting from the the TRP9 to GLY protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

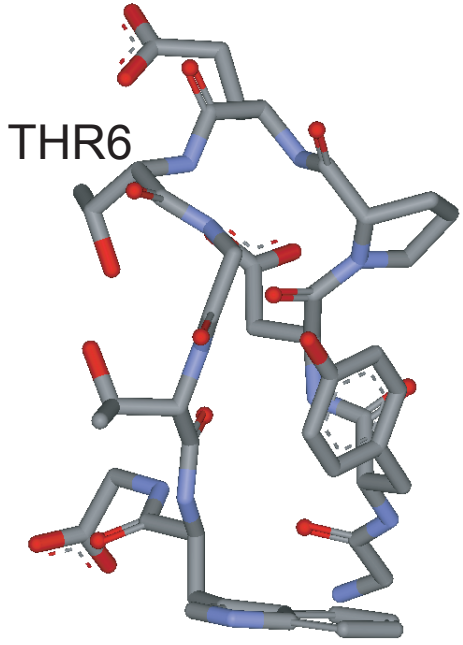
5. Repeat the similar simulations and report results for the TRP9 to THR protein mutation



# MM dynamics of small proteins (MM-44)

1. Perform energy minimization of Chignolin, starting from the the THR9 to TYR protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps




3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the THR9 to VAL protein mutation

# MM dynamics of small proteins (MM-45)

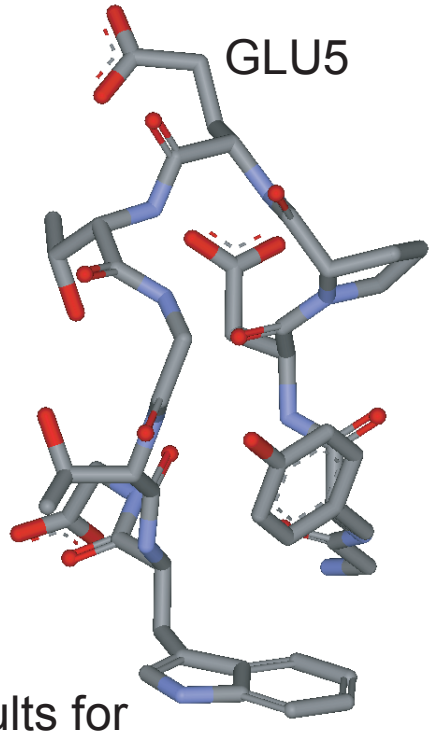
1. Perform energy minimization of Chignolin, starting from the the GLU5 to LYS protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the GLU5 to ASN protein mutation



# MM dynamics of small proteins (MM-46)

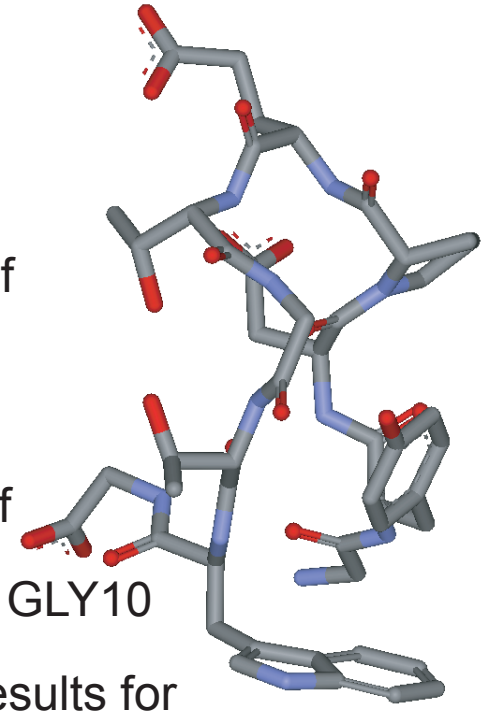
1. Perform energy minimization of Chignolin, starting from the the GLY10 to PHE protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the GLY10 to ILE protein mutation



GLY10

# MM dynamics of small proteins (MM-47)

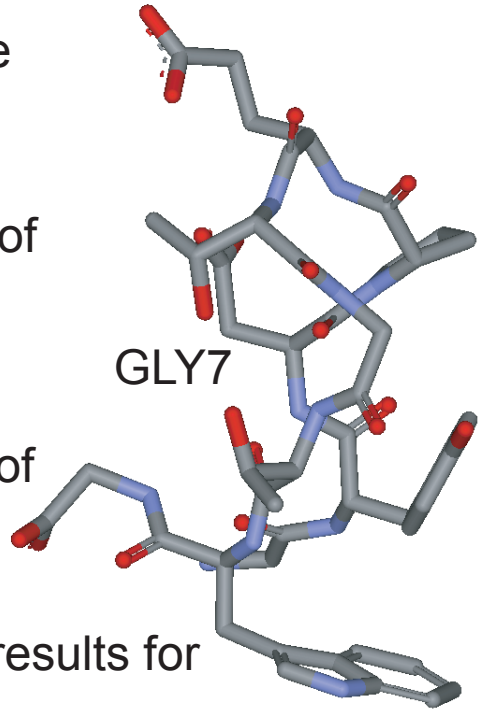
1. Perform energy minimization of Chignolin, starting from the the GLY7 to ARG protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the GLY7 to ALA protein mutation



# MM dynamics of small proteins (MM-48)

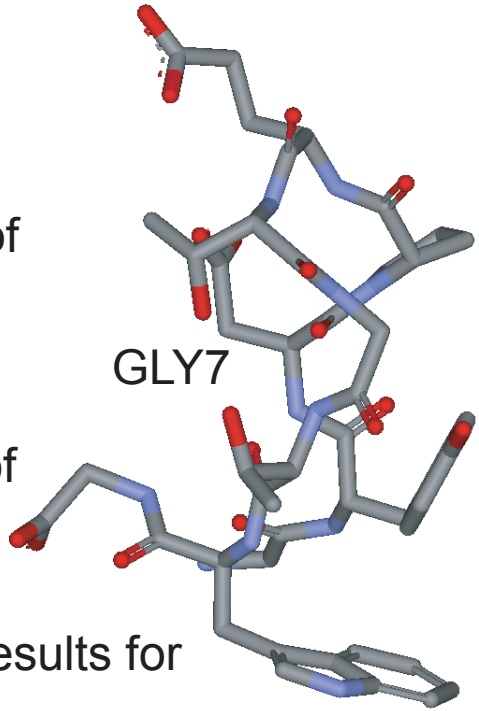
1. Perform energy minimization of Chignolin, starting from the GLY7 to SER protein mutation of the initial PDB file, using the AMBER force field

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the GLY7 to TYR protein mutation



# MM constrained dynamics of small proteins (MM-49)

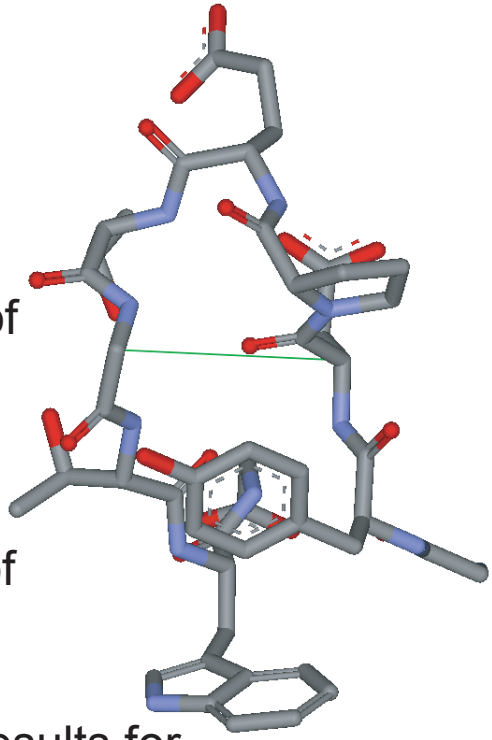
1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of GLY7 and CA of ASP3 of the value 8A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 10A



# MM constrained dynamics of small proteins (MM-50)

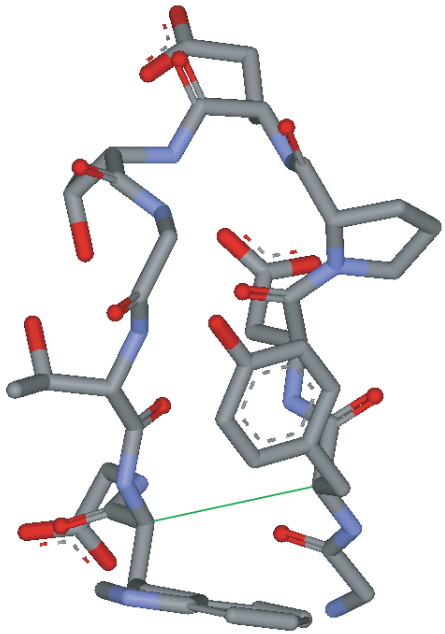
1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of TYR2 and CA of TRP9 of the value 6A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 12A

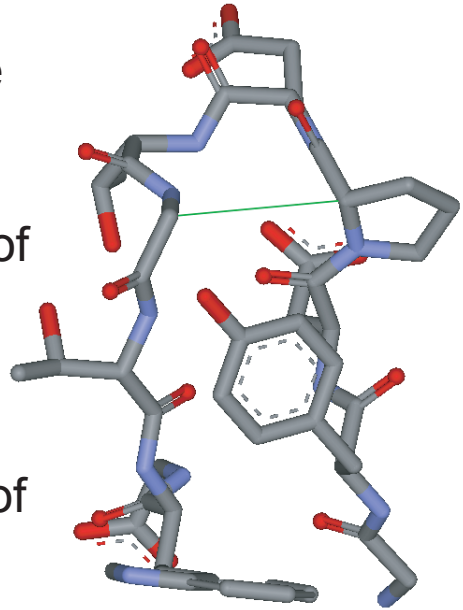


# MM constrained dynamics of small proteins (MM-51)

1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of PRO4 and CA of GLY7 of the value 5A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps



4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 10A

# MM constrained dynamics of small proteins (MM-52)

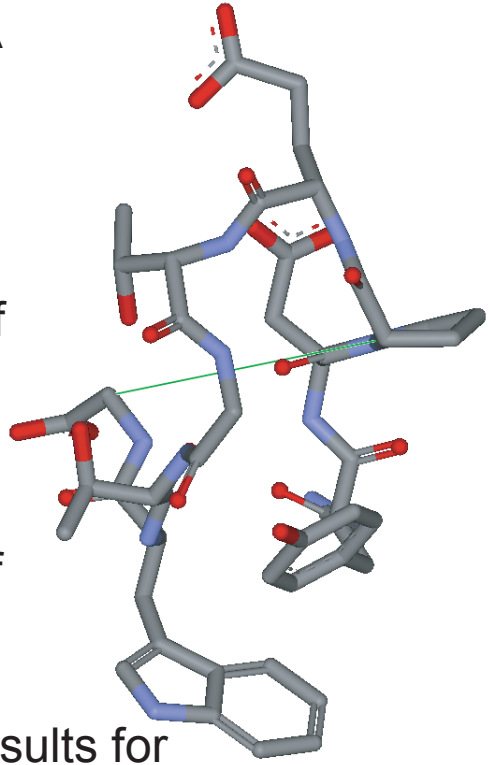
1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of PRO4 and CA of GLY10 of the value 10A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

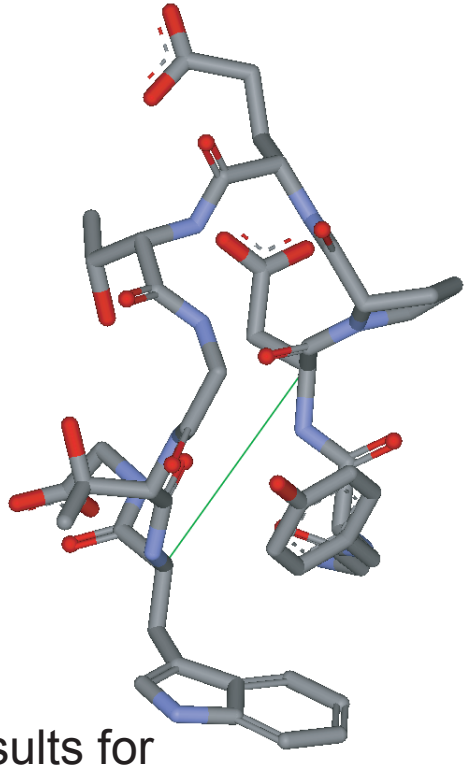
4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 15A



# MM constrained dynamics of small proteins (MM-53)

1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of ASP3 and CA of TRP9 of the value 6A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

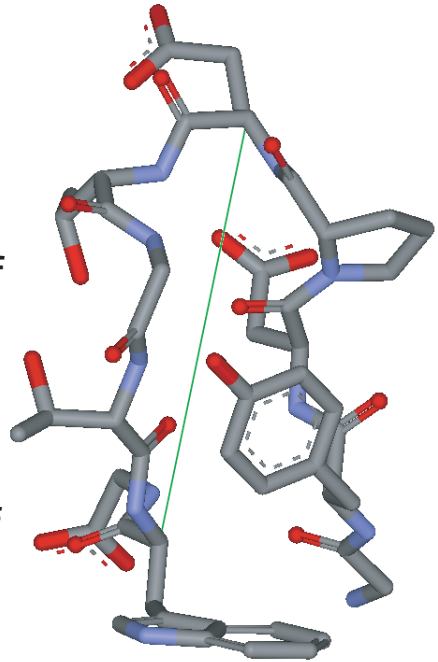
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 10A

# MM constrained dynamics of small proteins (MM-54)

1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of GLU5 and CA of TRP9 of the value 7A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

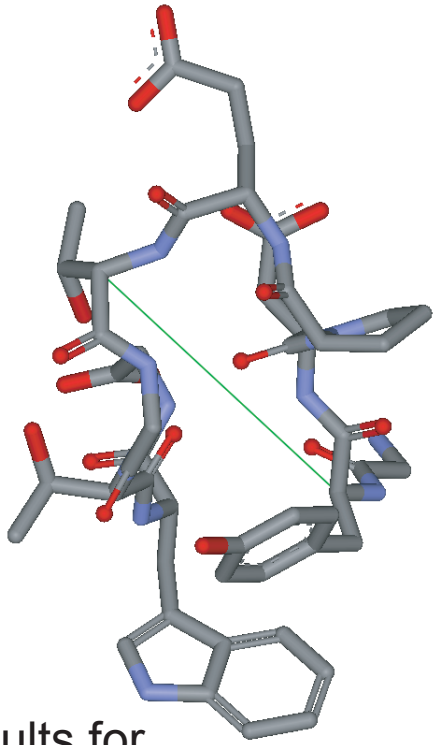
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 14A

# MM constrained dynamics of small proteins (MM-55)

1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of TYR2 and CA of THR6 of the value 8A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 12A

# MM constrained dynamics of small proteins (MM-56)

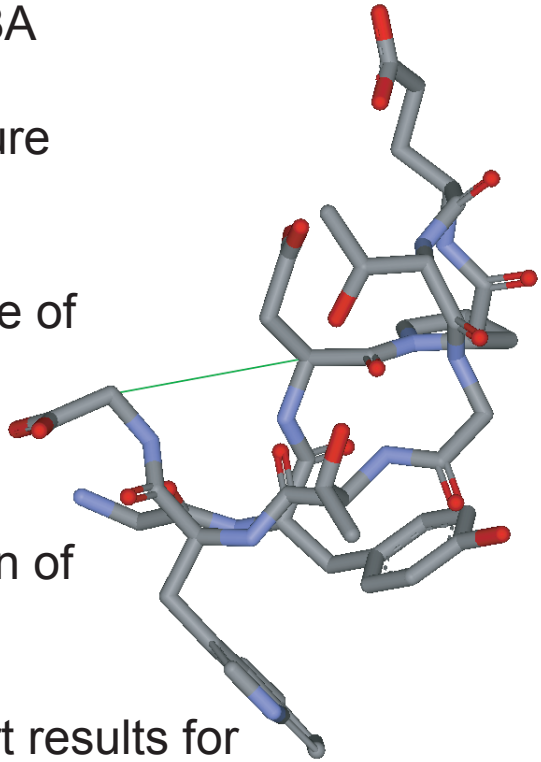
1. Perform energy minimization of Chignolin, starting from the the initial PDB file, and applying the constraint bewteen CA of ASP3 and CA of GLY10 of the value 8A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the constrined value of 14A



# MM dynamics of small proteins in a water sphere (MM-57)

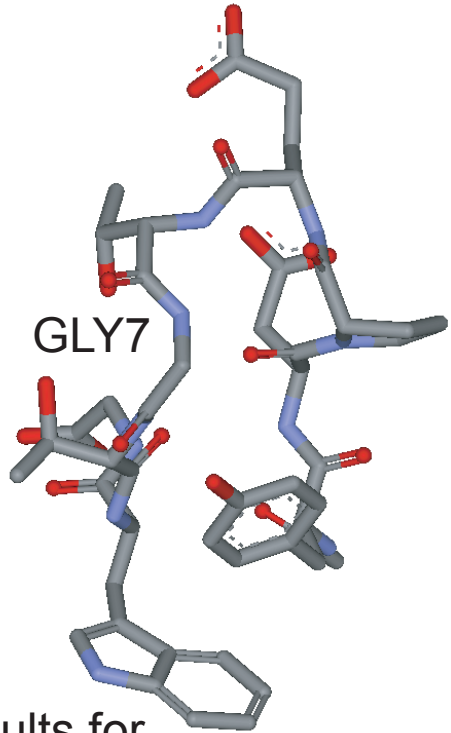
1. Perform energy minimization of Chignolin, starting from the GLY7 to GLU mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A



# MM dynamics of small proteins in a water sphere (MM-58)

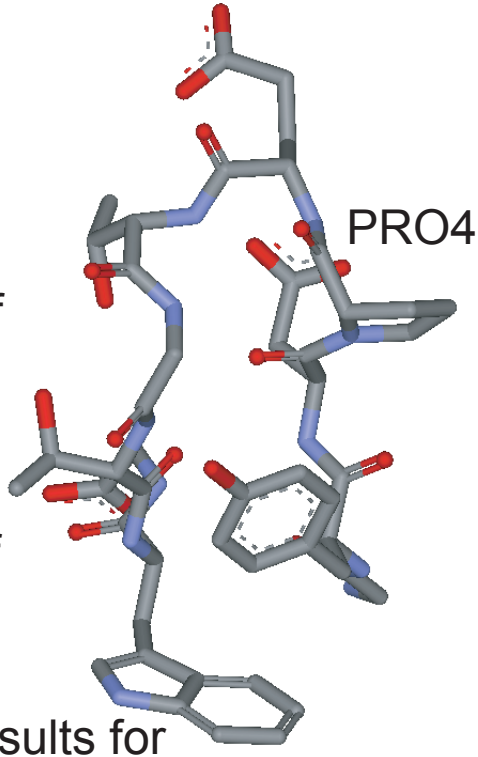
1. Perform energy minimization of Chignolin, starting from the PRO4 to ASP mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A



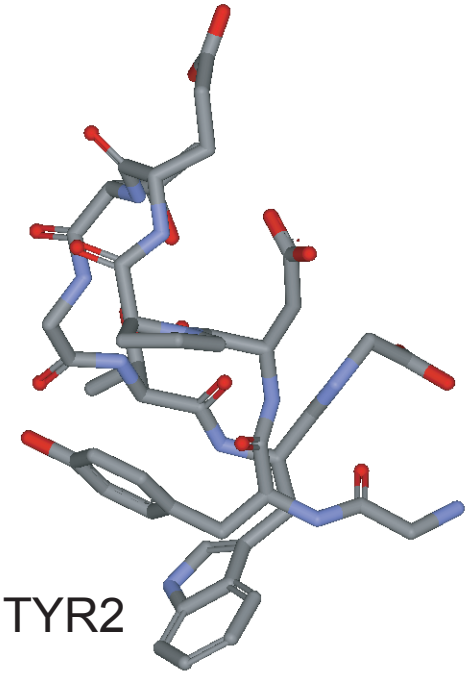
# MM dynamics of small proteins in a water sphere (MM-59)

1. Perform energy minimization of Chignolin, starting from the TYR2 to HIS(δ) mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time



TYR2

5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A

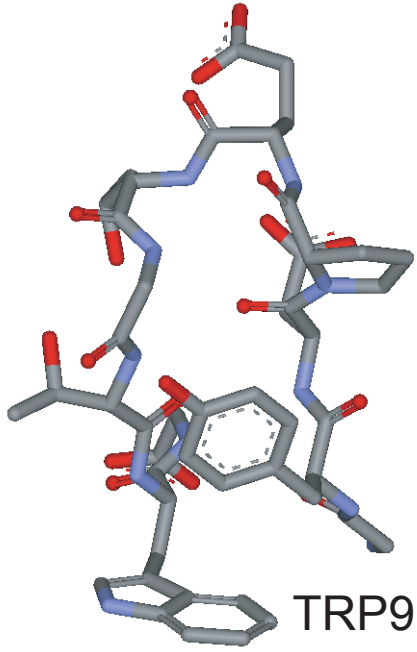
# MM dynamics of small proteins in a water sphere (MM-60)

1. Perform energy minimization of Chignolin, starting from the TRP9 to CYS mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time



TRP9

5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A

# MM dynamics of small proteins in a water sphere (MM-61)

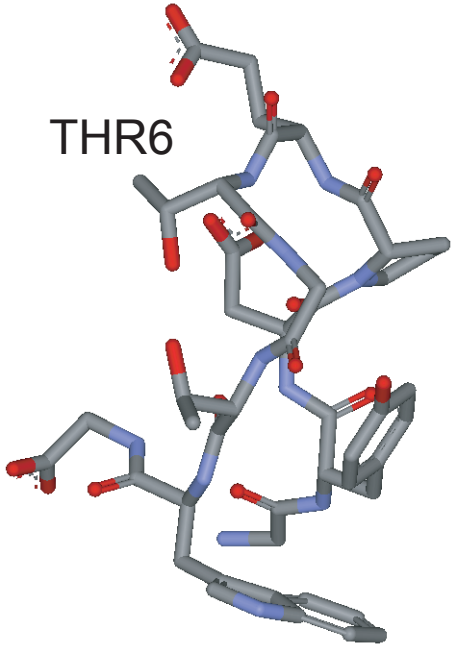
1. Perform energy minimization of Chignolin, starting from the THR6 to TYR mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A



# MM dynamics of small proteins in a water sphere (MM-62)

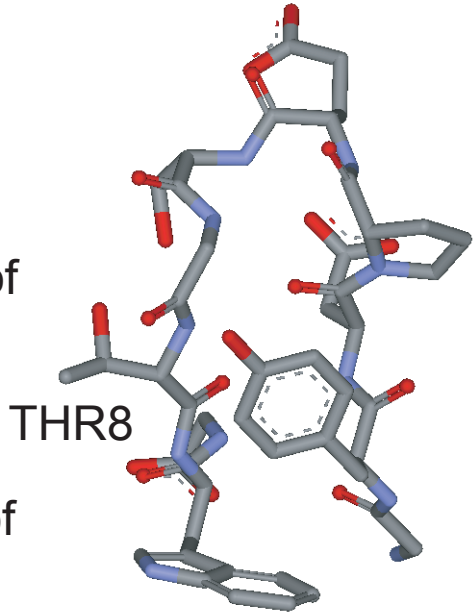
1. Perform energy minimization of Chignolin, starting from the THR8 to TRP mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A



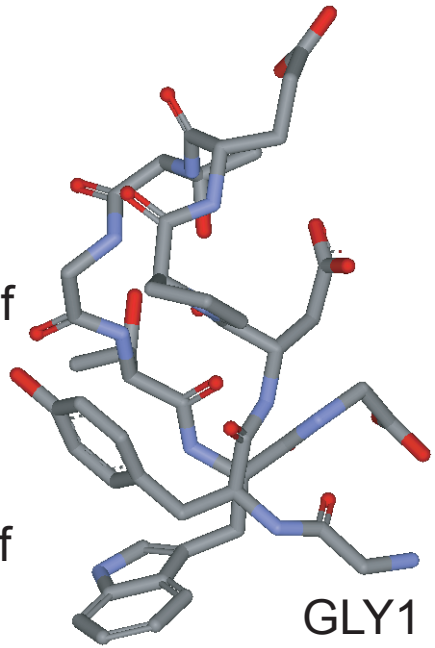
# MM dynamics of small proteins in a water sphere (MM-63)

1. Perform energy minimization of Chignolin, starting from the GLY1 to ARG mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time




5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A

# MM dynamics of small proteins in a water sphere (MM-64)

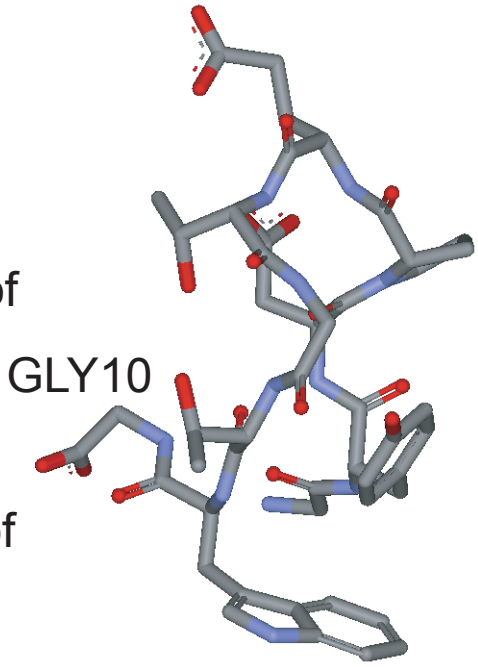
1. Perform energy minimization of Chignolin, starting from the GLY10 to PRO mutation of the initial PDB file, in a sphere of water molecules of a radius 20A

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the sphere of water molecules of a radius 30A



# MM dynamics of small proteins in a water box (MM-65)

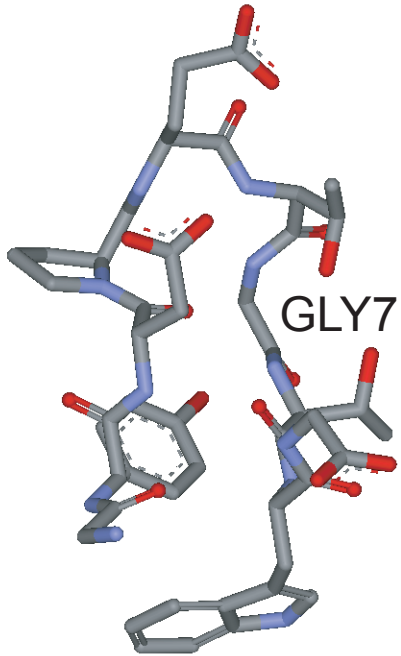
1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of GLY7

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees



# MM dynamics of small proteins in a water box (MM-66)

1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of PRO4

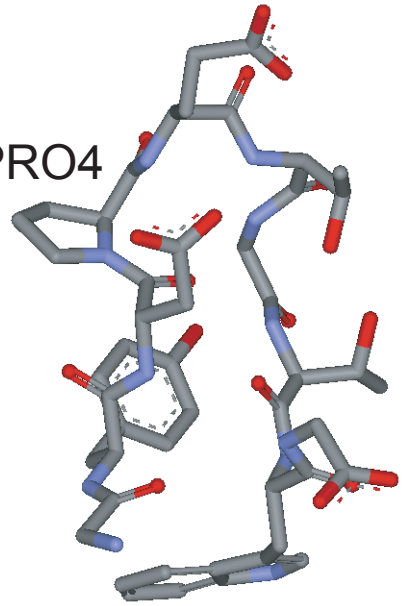
2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees

PRO4



# MM dynamics of small proteins in a water box (MM-67)

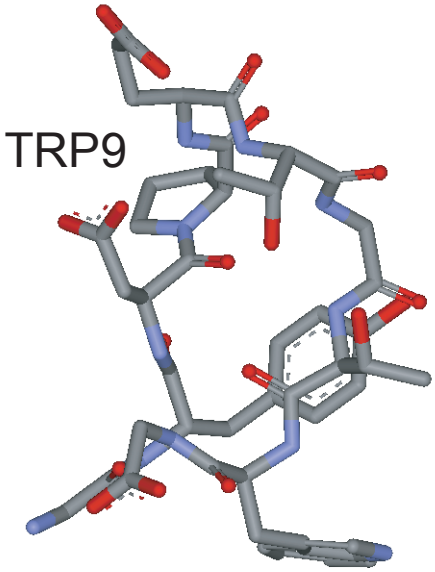
1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of TRP9

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees



# MM dynamics of small proteins in a water box (MM-68)

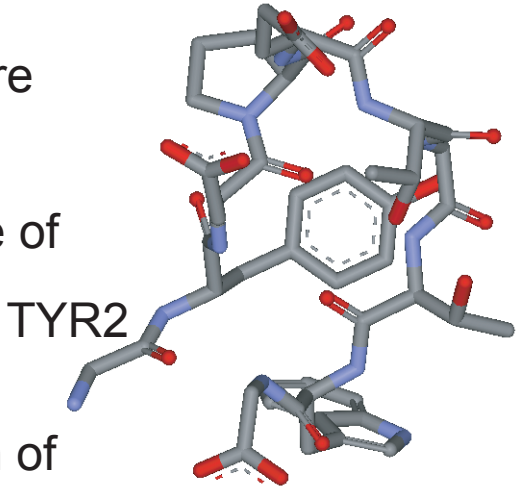
1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of TYR2

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees



# MM dynamics of small proteins in a water box (MM-69)

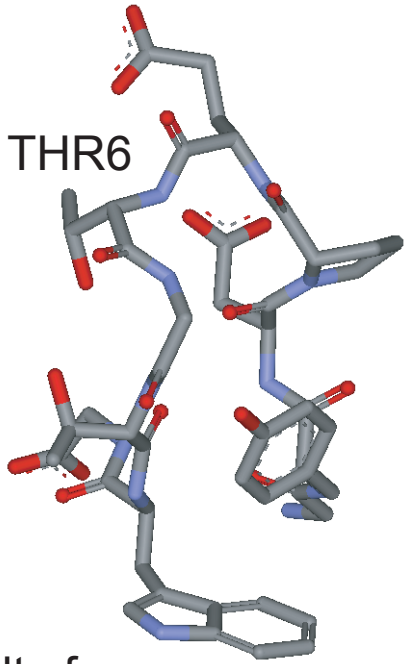
1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of THR6

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees



# MM dynamics of small proteins in a water box (MM-70)

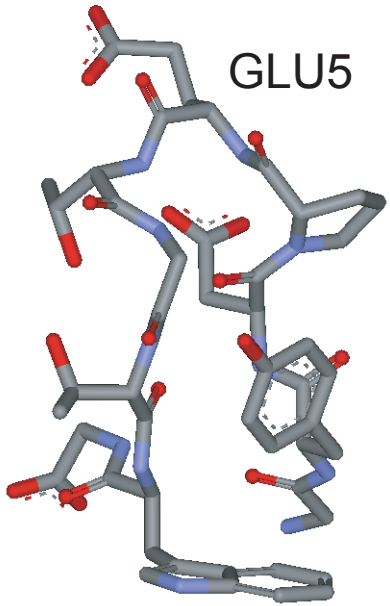
1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of GLU5

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees



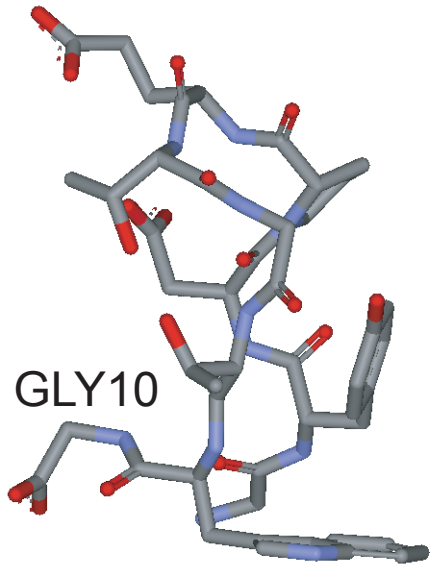
# MM dynamics of small proteins in a water box (MM-71)

1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of GLY10

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time




5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees

# MM dynamics of small proteins in a water box (MM-72)

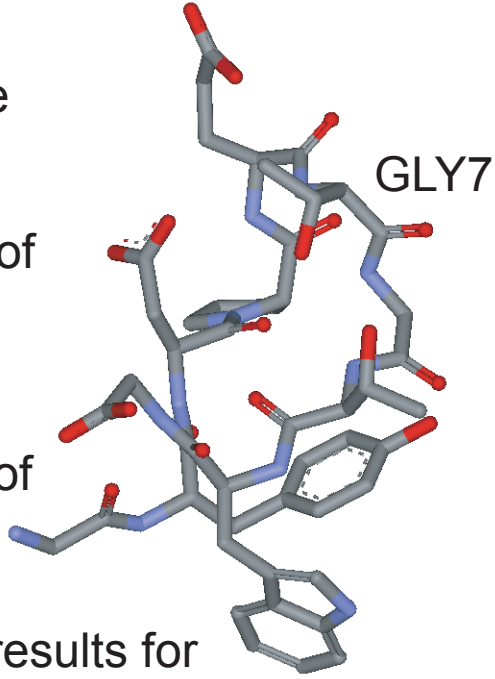
1. Perform energy minimization of Chignolin, starting from the initial PDB file, in a periodic box of water molecules, applying the torsional constraint of a value 180 degrees bewteen CA and N atoms of GLY7

2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

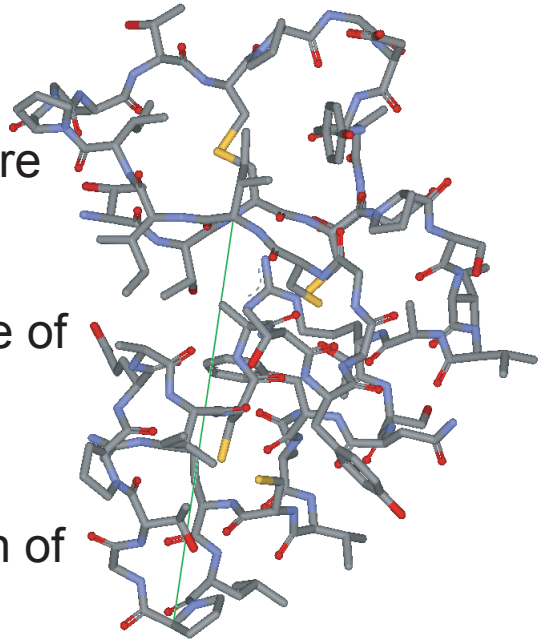
4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for the torsional constraint of a value 0 degrees



# MM dynamics of medium proteins in water sphere (MM-73)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 10A between PRO19 and ILE33in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

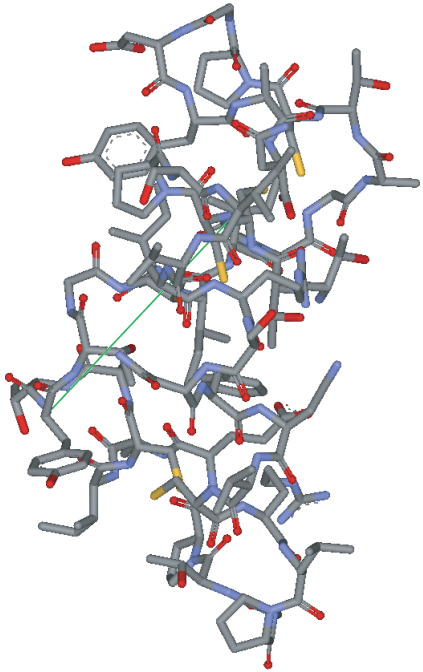
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A

# MM dynamics of medium proteins in water sphere (MM-74)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 10A between ILE7 and TYR29 in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

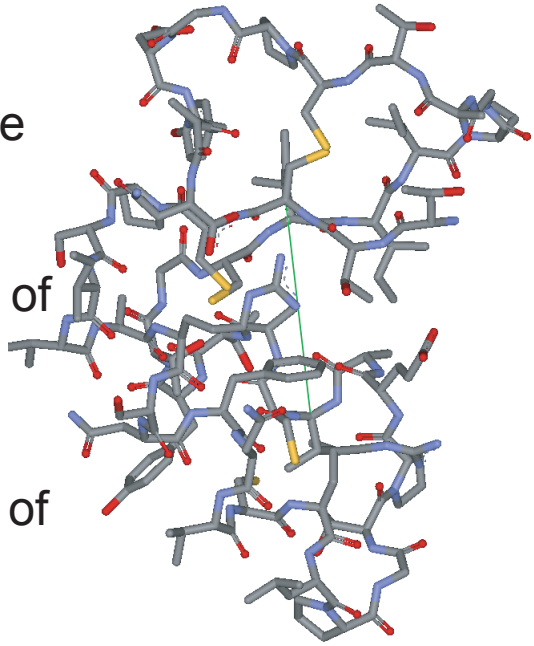
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A

# MM dynamics of medium proteins in water sphere (MM-75)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 10A between CYS3 and ILE25 in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

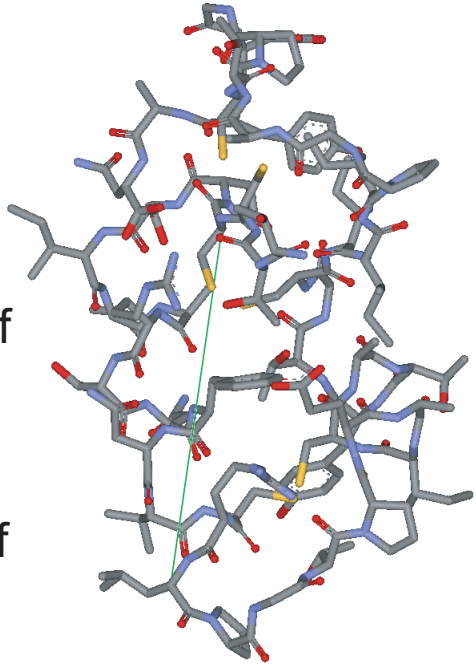
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A

# MM dynamics of medium proteins in water sphere (MM-76)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 10A between CYS4 and LEU18 in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

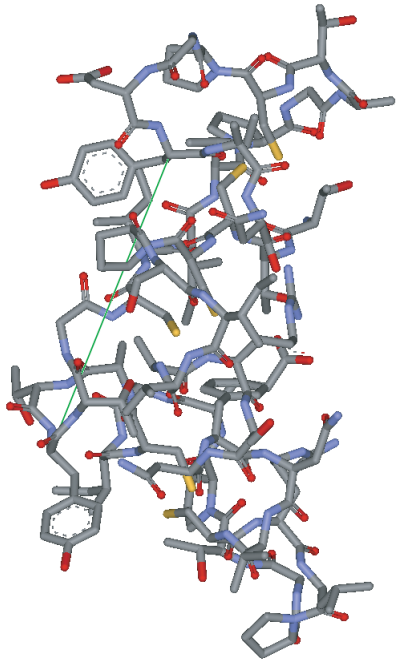
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A

# MM dynamics of medium proteins in water sphere (MM-77)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 10A between TYR29 and TYR44 in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

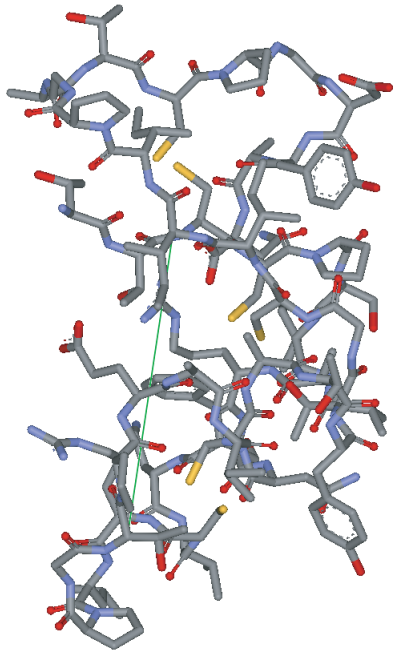
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A

# MM dynamics of medium proteins in water sphere (MM-78)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 10A between THR21 and ILE34 in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

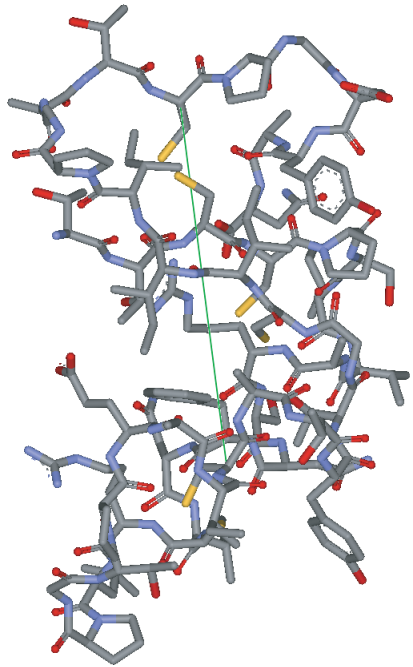
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A

# MM dynamics of medium proteins in water sphere (MM-79)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 10A between CYS26 and CYS40 in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

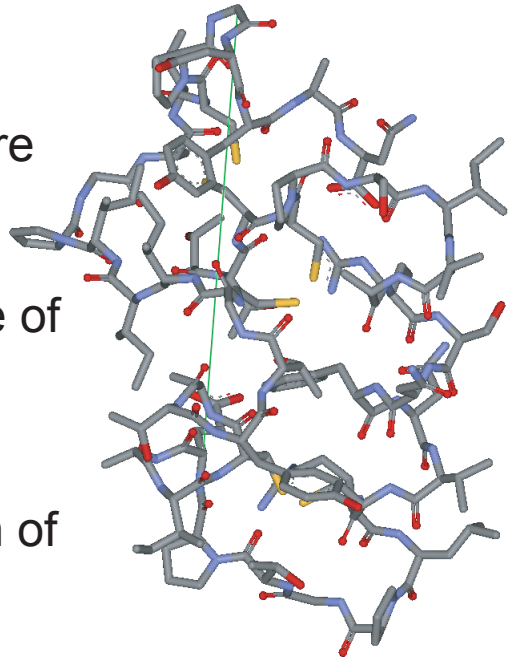
3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A

# MM dynamics of medium proteins in water sphere (MM-80)

1. Perform energy minimization of Crambin, starting from the the initial PDB file, applying a CA-CA distance constraint of a value 20A between GLU23 and GLY42 in a sphere of water molecules of a radius 30A



2. Perform heating of the minimized structure of the protein, from 0K to 300K for 20ps

3. Perform dynamics of the heated structure of the protein for 500ps

4. Report in a figure the total energy of the protein and the temperature as a function of the dynamics time

5. Repeat the similar simulations and report results for distance constraint of a value 15A