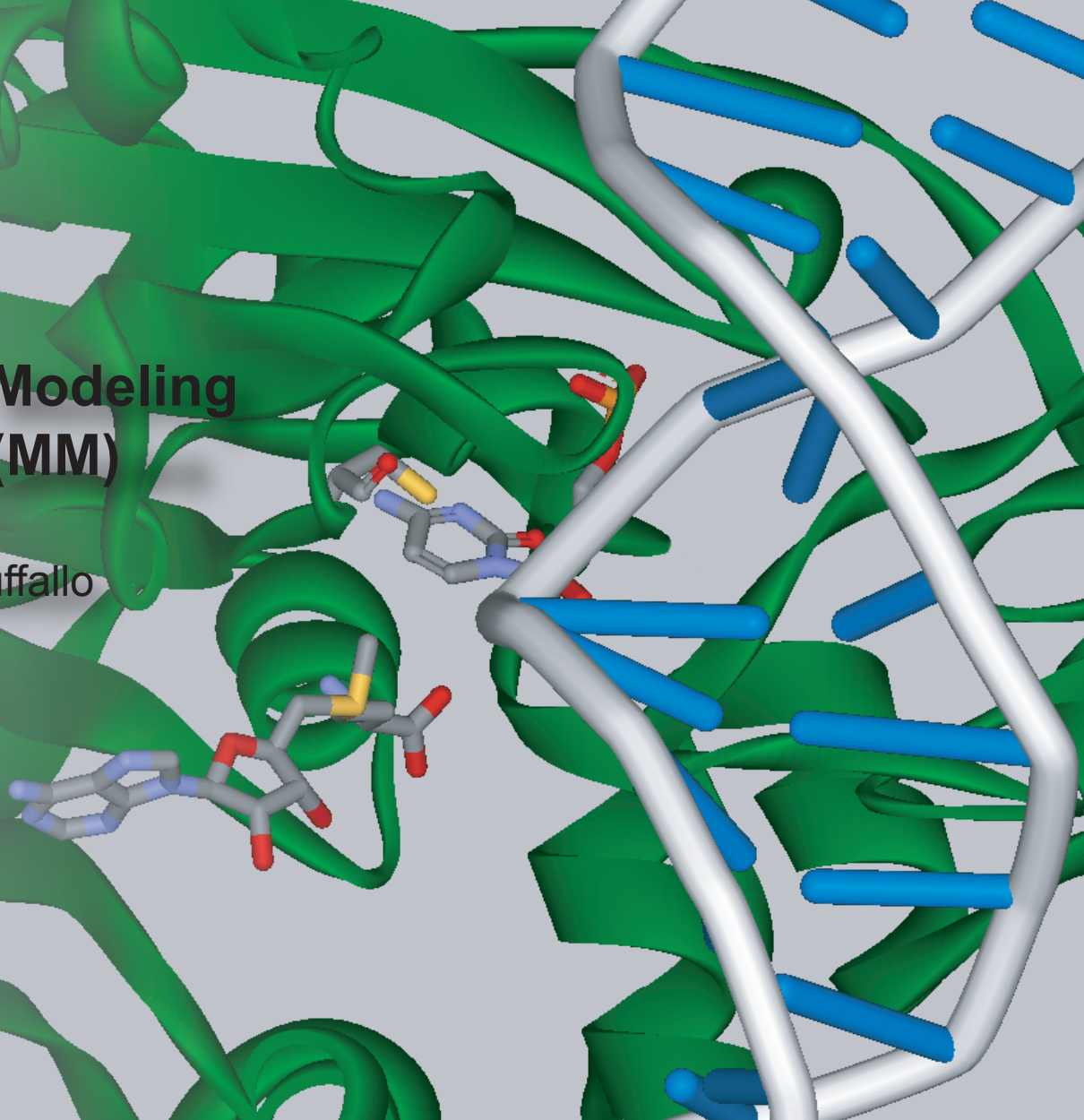


Marek
Freindorf

Molecular Modeling Examples (MM)

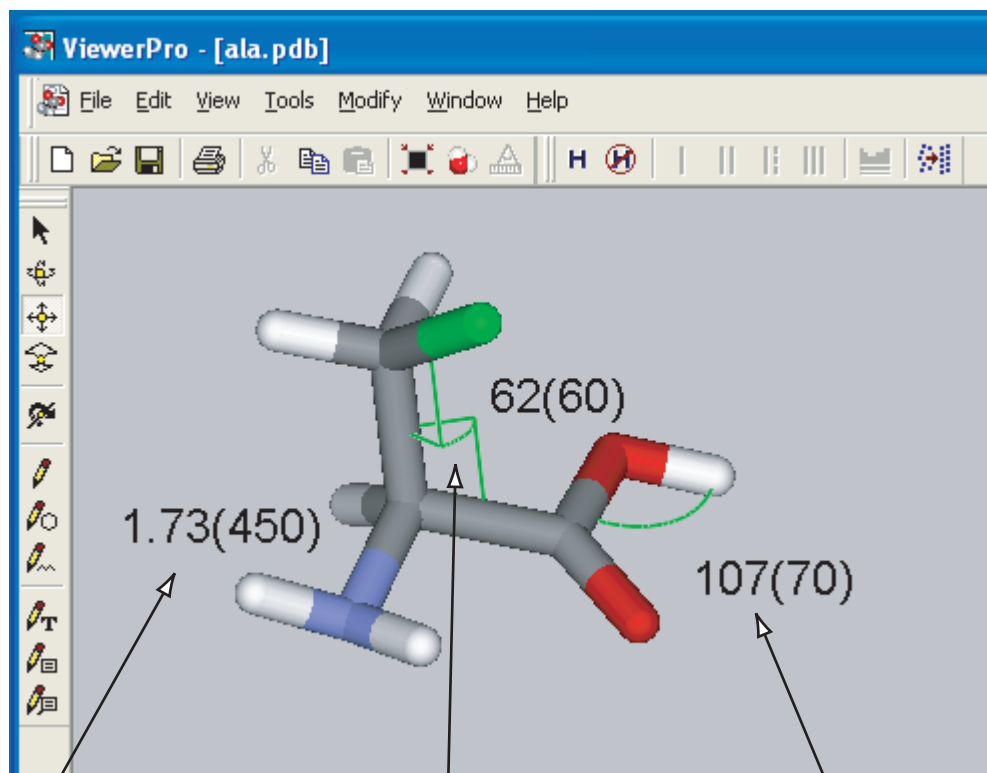
University at Buffalo
June 2006



MM parameters

Bonded parameters are related to bonding interactions between atoms

- Stretching
- Bending
- Torsion



Distance
(force constant)

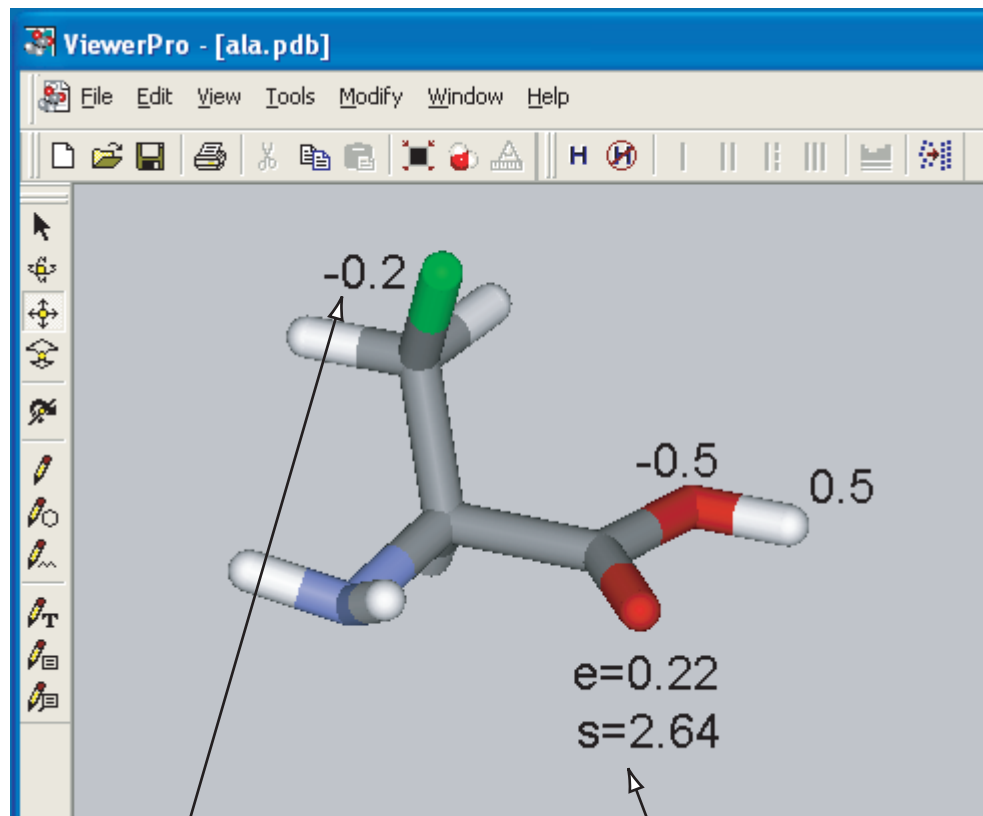
Torsion
(force constant)

Angle
(force constant)

MM parameters

Non-bonded parameters are related to non-bonding interactions between atoms:

- Electrostatic
- Steric



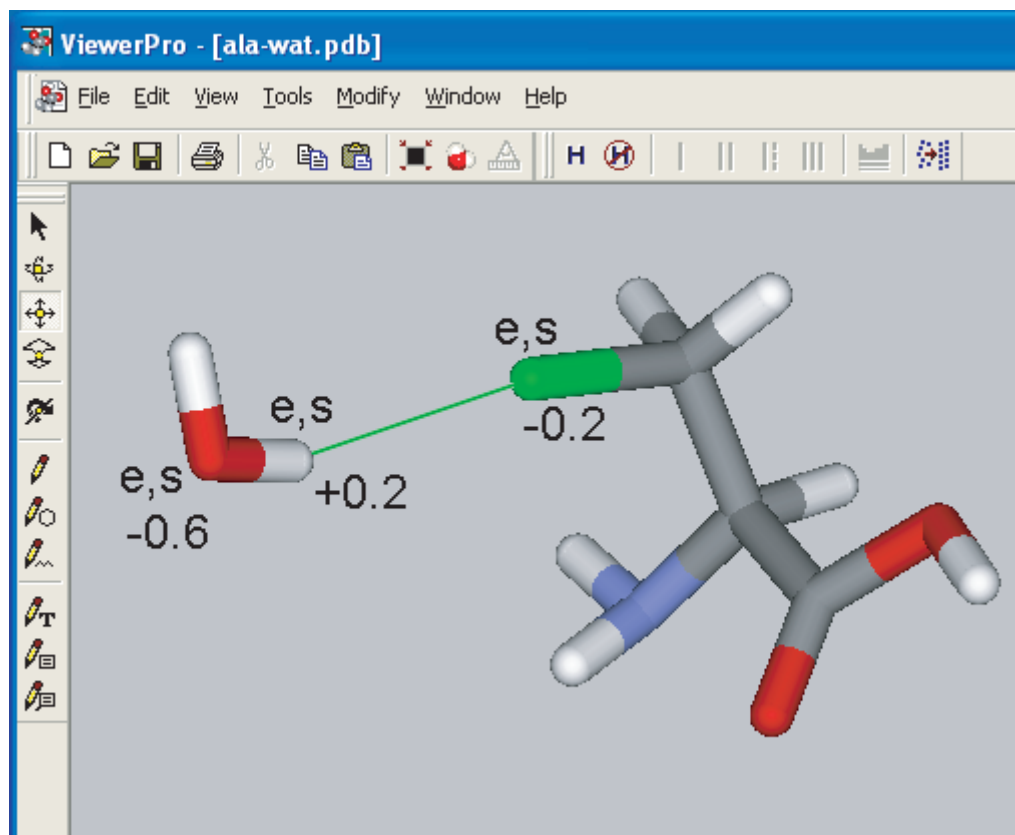
Atomic
charges

Van der Waals
sigma and epsilon

MM parameters

Hydrogen bonding interactions are combination of

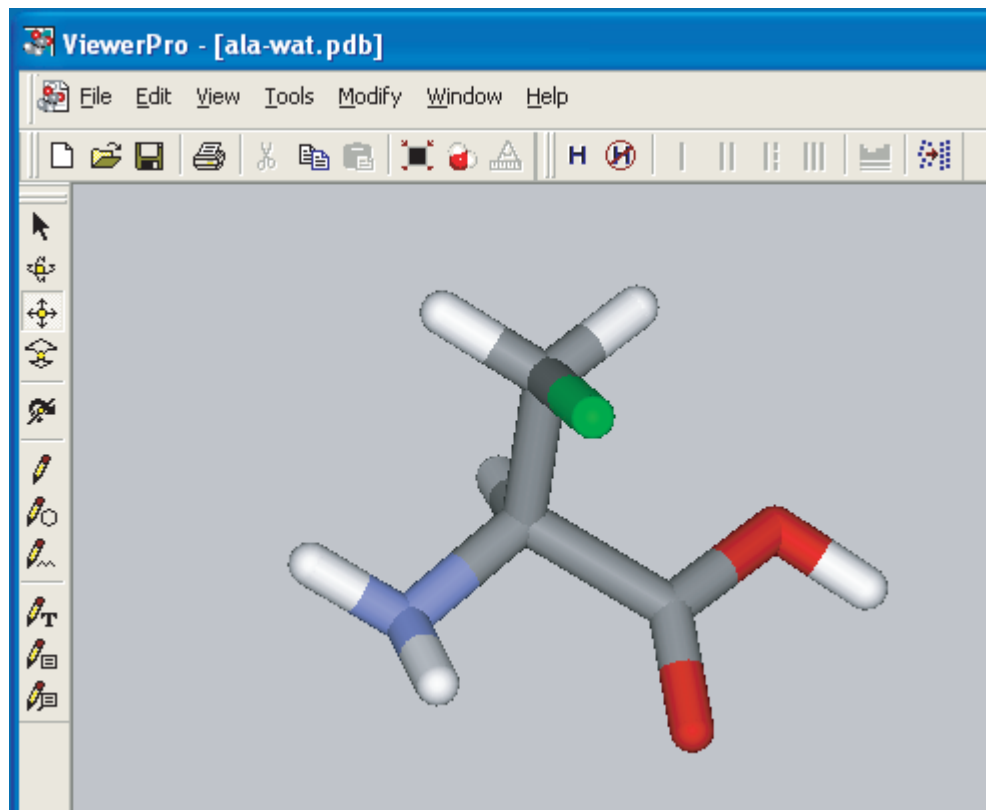
- Electrostatic
- Steric



MM parameters

Three methods
of evaluation
MM parameters

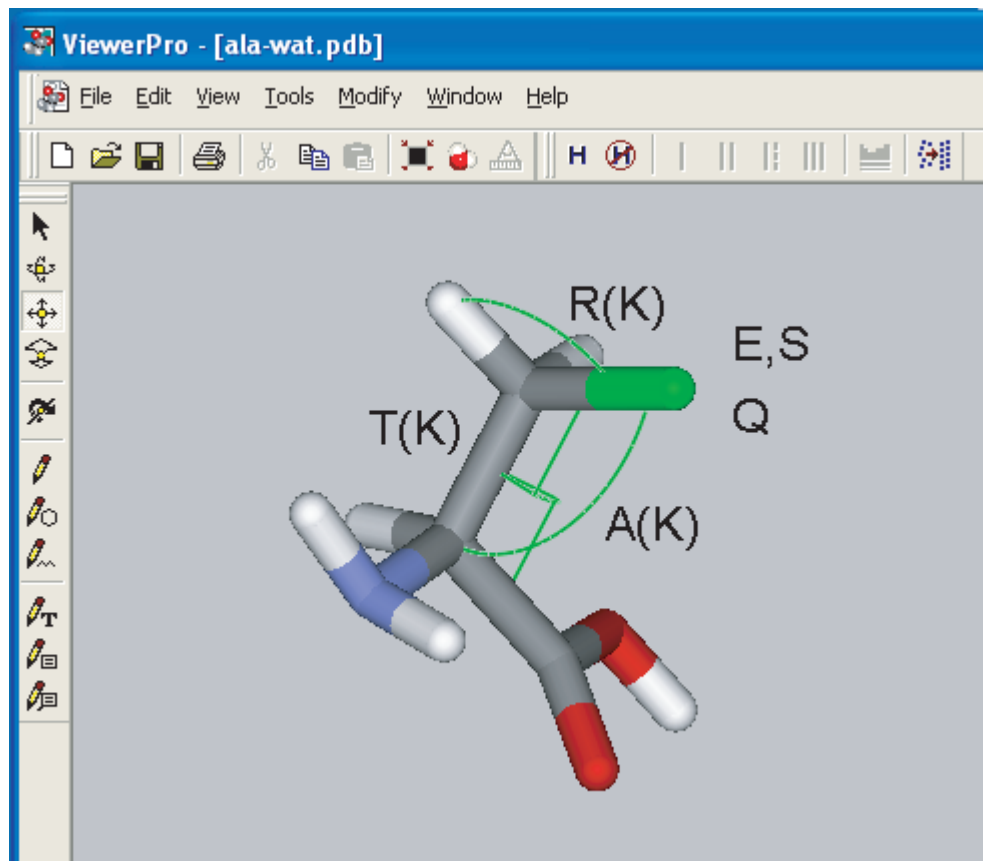
- QM calculations
- Experiment
- Analogy



MM parameters (Chloro-alanine)

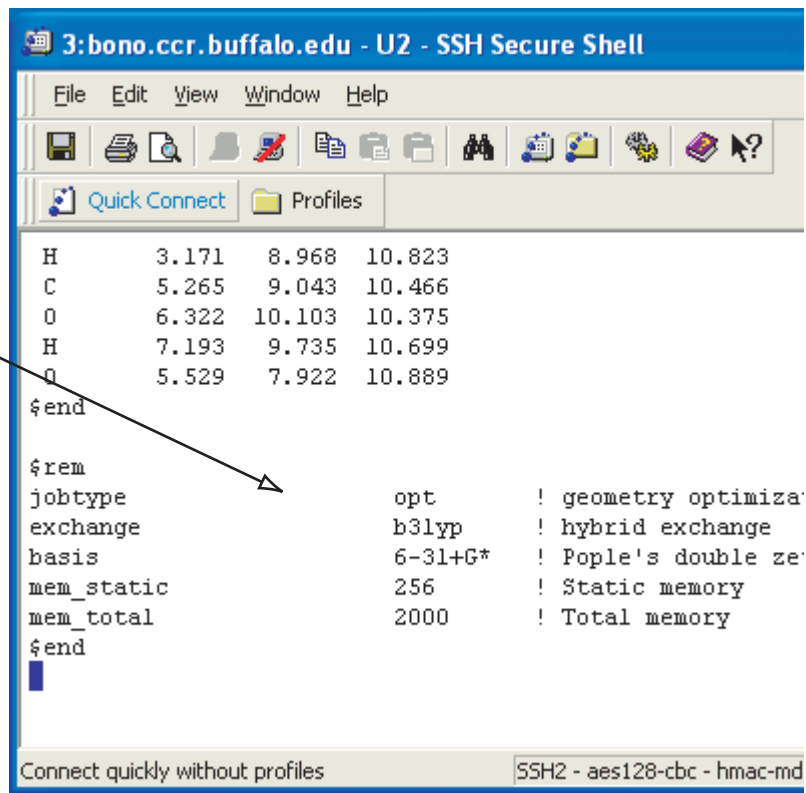
New atom

- Distances (Cons.)
- Angles (Const.)
- Torsions (Const.)
- Charge
- Van der Waals



MM parameters (Chloro-alanine)

QM geometry
optimization of the
molecule in the gas
phase



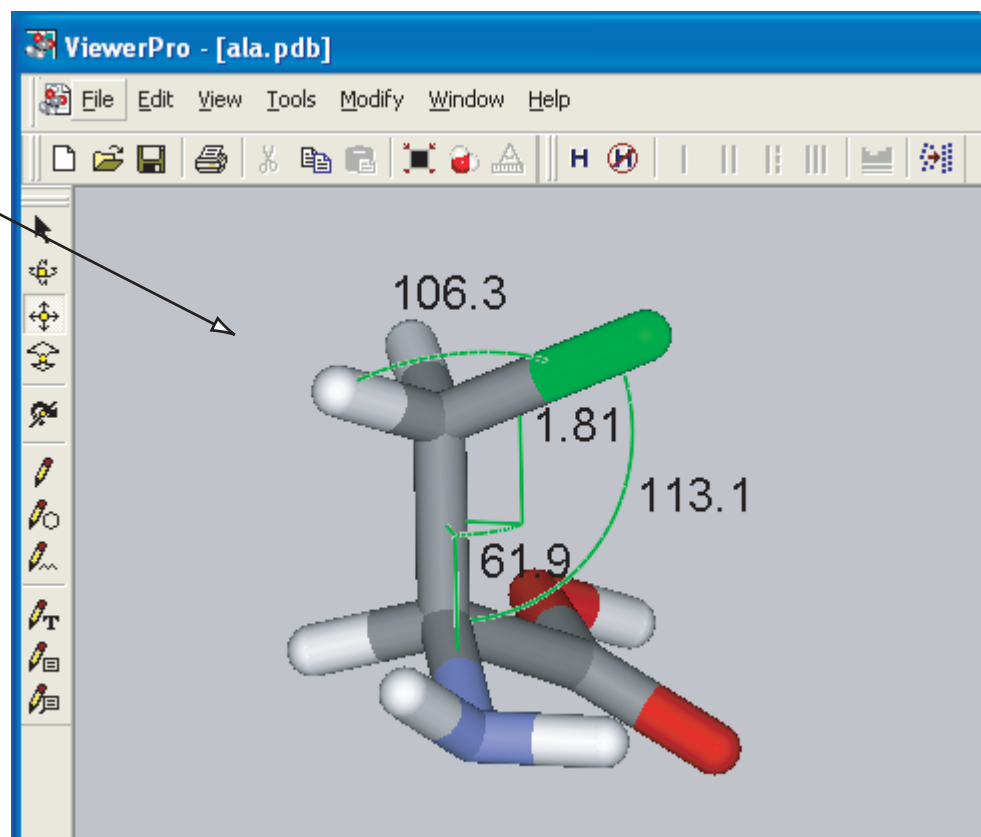
```
3:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
H      3.171   8.968  10.823
C      5.265   9.043  10.466
O      6.322  10.103  10.375
H      7.193   9.735  10.699
O      5.529   7.922  10.889
$end

$rem
jobtype                opt          ! geometry optimization
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double zeta
mem_static             256          ! Static memory
mem_total              2000         ! Total memory
$end
█

Connect quickly without profiles  SSH2 - aes128-cbc - hmac-md5
```

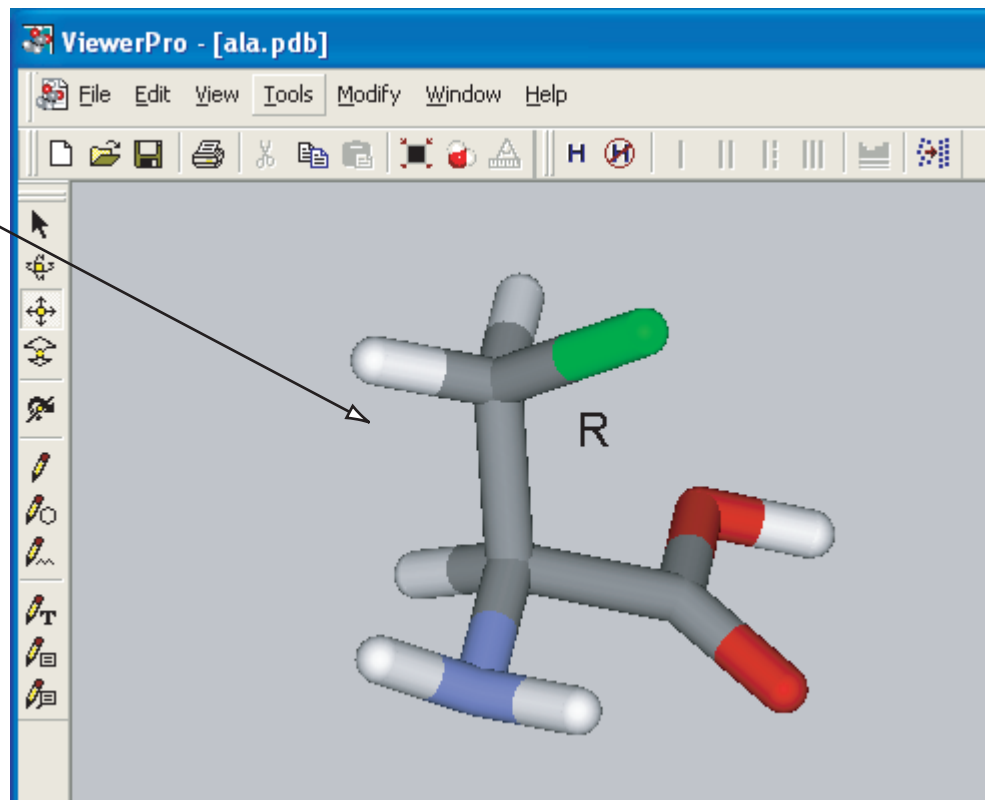

MM parameters (Chloro-alanine)

Results of the
calculations



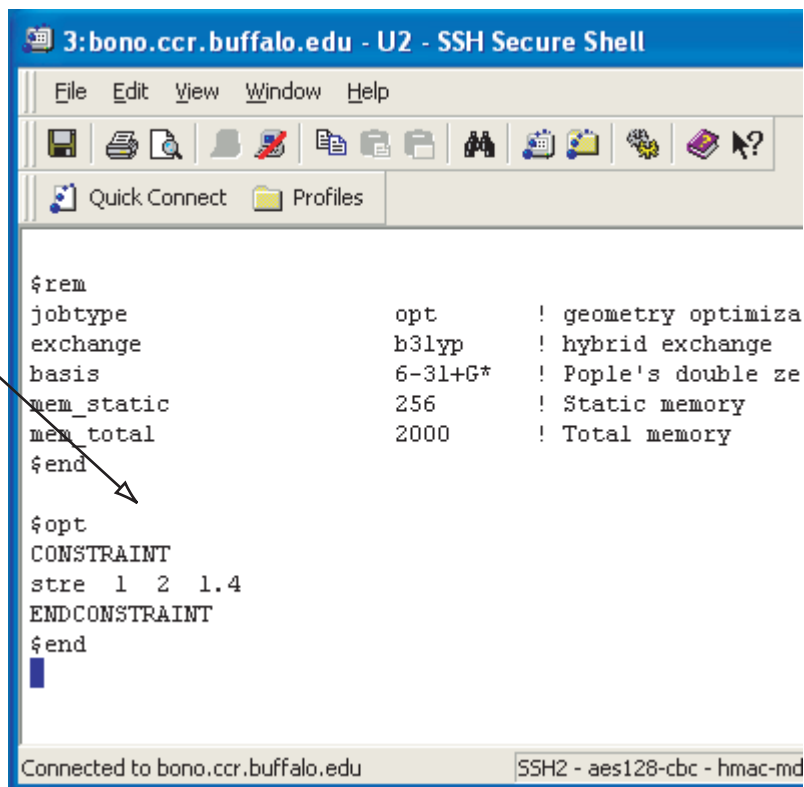
MM parameters (Chloro-alanine)

Calculations of the optimal geometry with a fixed interatomic distance



MM parameters (Chloro-alanine)

Constrained interatomic distance



```
3:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

$rem
jobtype                opt          ! geometry optimiza
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double ze
mem_static             256          ! Static memory
mem_total              2000         ! Total memory
$end

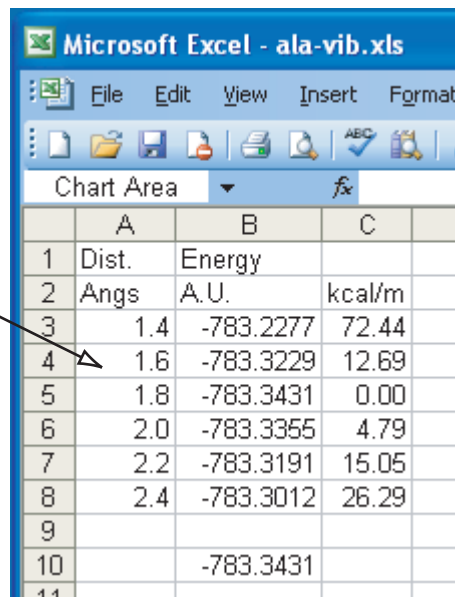
$opt
CONSTRAINT
stre 1 2 1.4
ENDCONSTRAINT
$end

[Cursor]
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md

MM parameters (Chloro-alanine)

Results of the
calculations



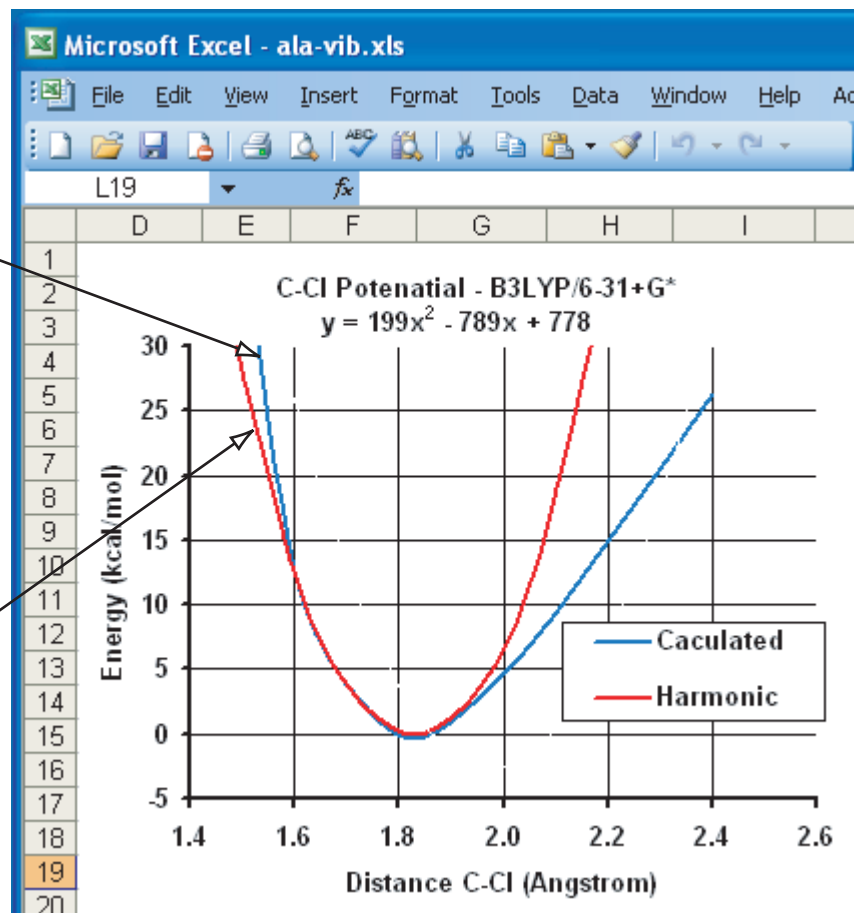
	A	B	C
1	Dist.	Energy	
2	Angs	A.U.	kcal/m
3	1.4	-783.2277	72.44
4	1.6	-783.3229	12.69
5	1.8	-783.3431	0.00
6	2.0	-783.3355	4.79
7	2.2	-783.3191	15.05
8	2.4	-783.3012	26.29
9			
10		-783.3431	
11			

MM parameters (Chloro-alanine)

Potential energy
surface of the C-Cl
stretching

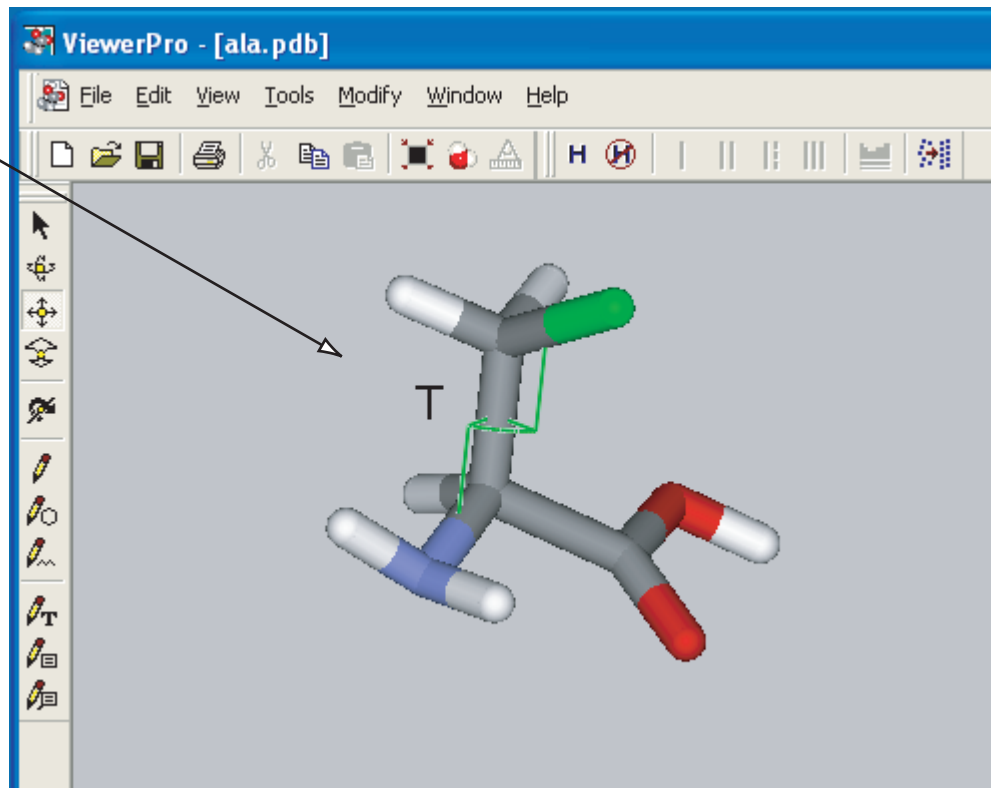
Harmonic
approximation:

$$E = \frac{1}{2} K (q - q_0)^2$$



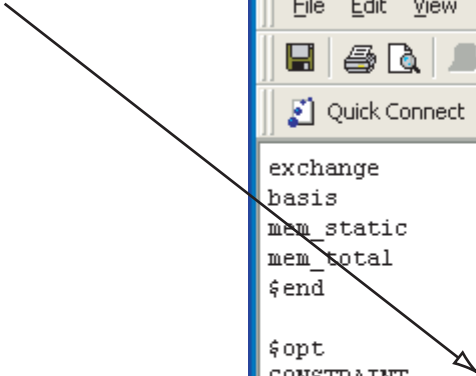
MM parameters (Chloro-alanine)

Geometry
optimization with a
constrained torsion
angle



MM parameters (Chloro-alanine)

Geometry
optimization with a
constrained torsion
angle



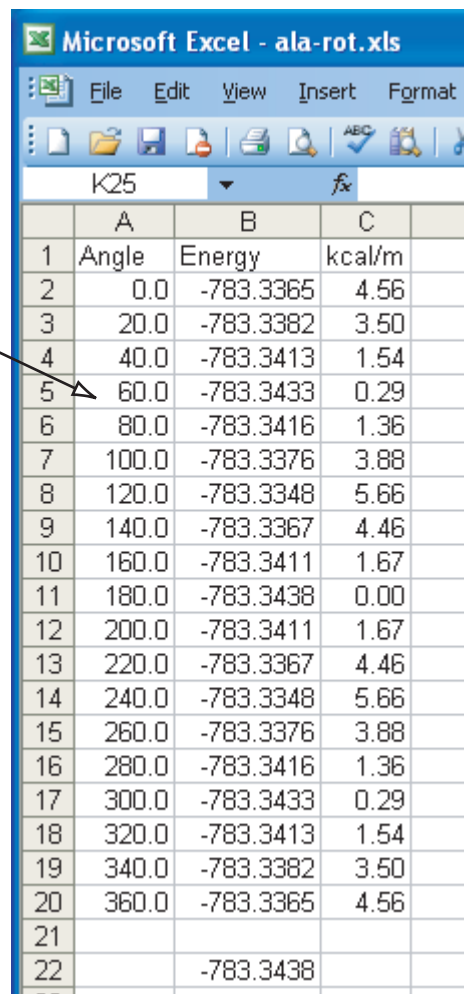
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
exchange          b3lyp      ! hybrid exchange
basis             6-31+G*   ! Pople's double zet
mem_static        256       ! Static memory
mem_total         2000      ! Total memory
$end

$opt
CONSTRAINT
tors 1 2 5 6 100.0
ENDCONSTRAINT
$end
█

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```

MM parameters (Chloro-alanine)

Results of the
calculations



Microsoft Excel - ala-rot.xls

File Edit View Insert Format

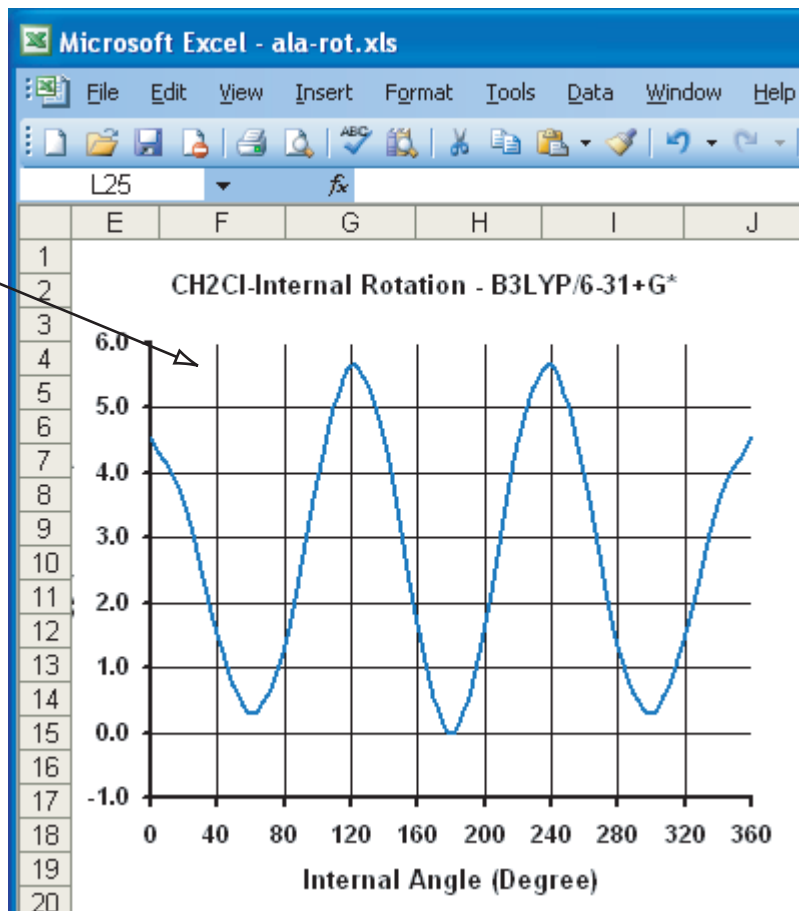
K25

	A	B	C
1	Angle	Energy	kcal/m
2	0.0	-783.3365	4.56
3	20.0	-783.3382	3.50
4	40.0	-783.3413	1.54
5	60.0	-783.3433	0.29
6	80.0	-783.3416	1.36
7	100.0	-783.3376	3.88
8	120.0	-783.3348	5.66
9	140.0	-783.3367	4.46
10	160.0	-783.3411	1.67
11	180.0	-783.3438	0.00
12	200.0	-783.3411	1.67
13	220.0	-783.3367	4.46
14	240.0	-783.3348	5.66
15	260.0	-783.3376	3.88
16	280.0	-783.3416	1.36
17	300.0	-783.3433	0.29
18	320.0	-783.3413	1.54
19	340.0	-783.3382	3.50
20	360.0	-783.3365	4.56
21			
22		-783.3438	

MM parameters (Chloro-alanine)

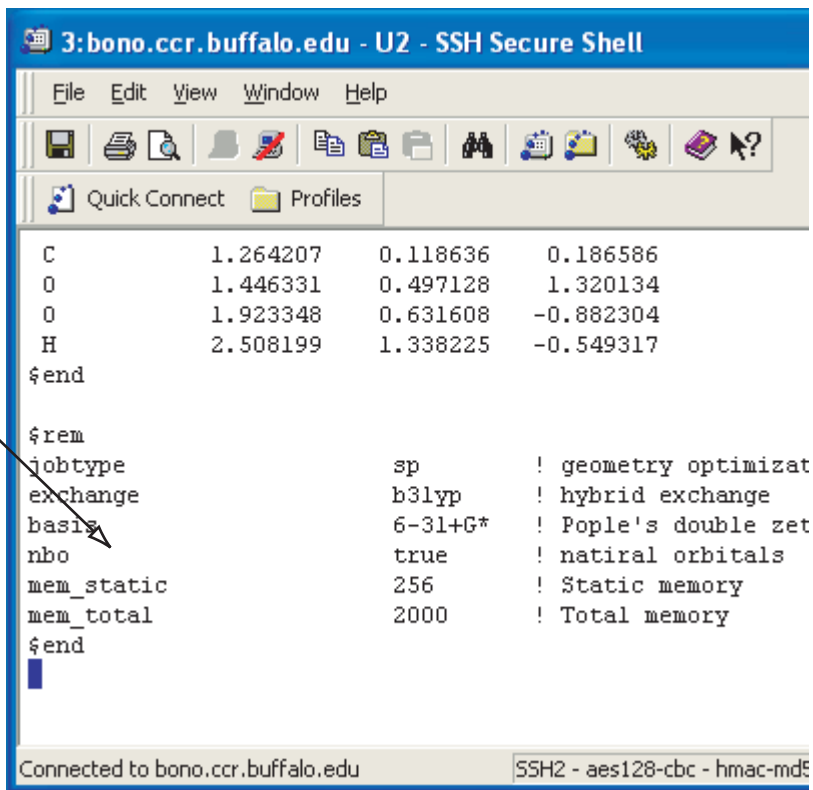
Potential energy surface of the internal rotation

- Angle at the minimum
- Energy at the maximum
- Number of maxima



MM parameters (Chloro-alanine)

Calculations of natural
orbitals



```
3:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
C      1.264207    0.118636    0.186586
O      1.446331    0.497128    1.320134
O      1.923348    0.631608   -0.882304
H      2.508199    1.338225   -0.549317
$end

$rem
jobtype          sp          ! geometry optimizat
exchange         b3lyp        ! hybrid exchange
basis            6-31+G*      ! Pople's double zet
nbo              true         ! natural orbitals
mem_static       256          ! Static memory
mem_total       2000          ! Total memory
$end
█















Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```




MM parameters (Chloro-alanine)

Atomic charges
calculated using
natural orbitals

3:bono.ccr.buffalo.edu - U2 - SSH Secure Shell

FileEditViewWindowHelp



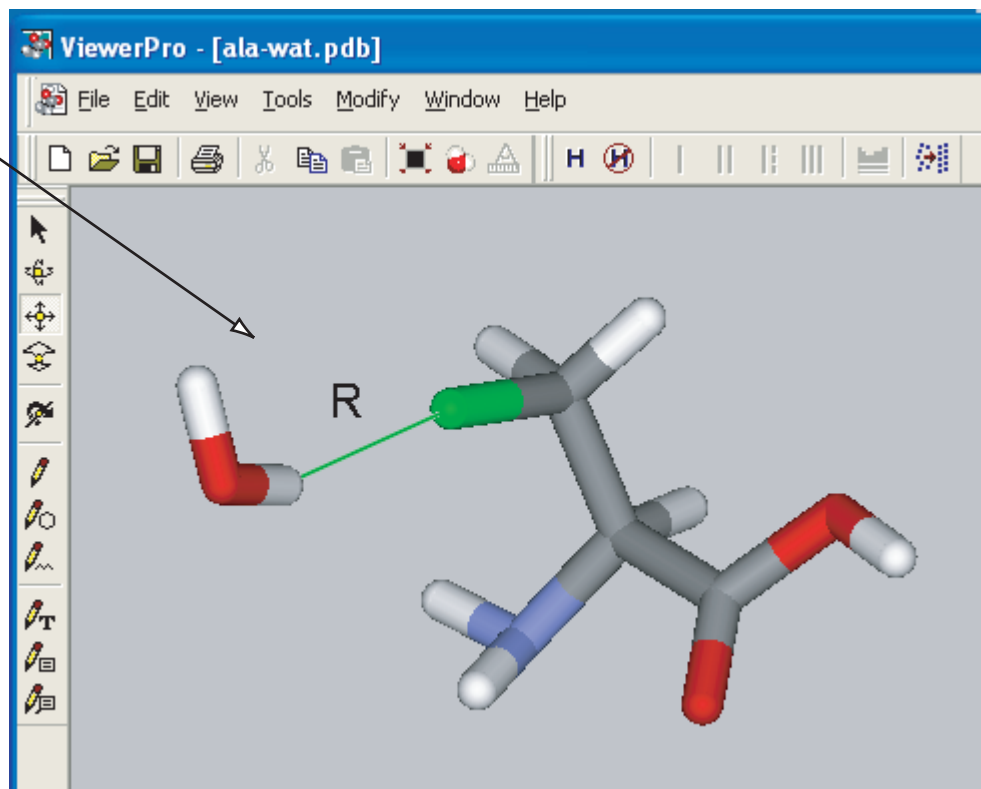
 Quick Connect Profiles

		Natural Charge	Natural Population		
Atom No			Core	Valence	Rydberg
Cl	1	-0.07967	9.99975	7.06270	0.01722
C	2	-0.45593	1.99922	4.44025	0.01645
H	3	0.27149	0.00000	0.72718	0.00133
H	4	0.25751	0.00000	0.74128	0.00121
C	5	-0.19245	1.99911	4.17113	0.02221
N	6	-0.90967	1.99963	5.88223	0.02781
H	7	0.39422	0.00000	0.60480	0.00098
H	8	0.41695	0.00000	0.58166	0.00138
H	9	0.27417	0.00000	0.72459	0.00124
C	10	0.81668	1.99941	3.13497	0.04895

Connected to bono.ccr.buffalo.eduSSH2 - aes128-cbc - hmac-md5 -

MM parameters (Chloro-alanine)

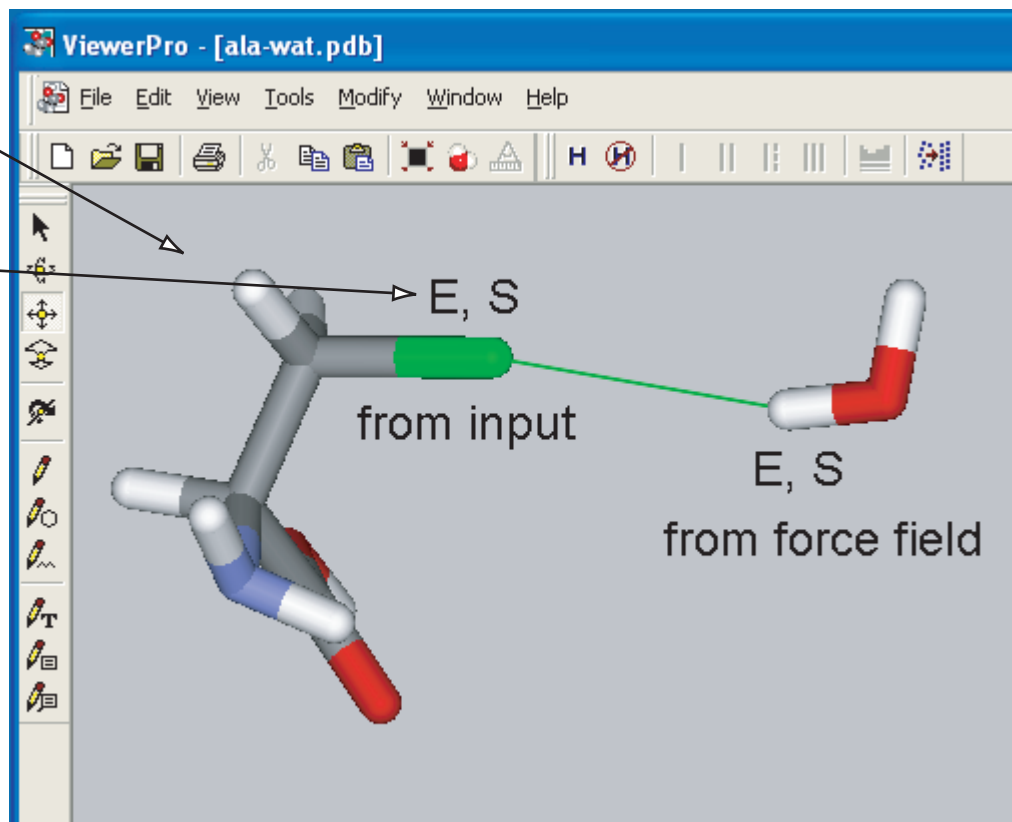
QM calculations of
a dimer with a
water molecule



MM parameters (Chloro-alanine)

Geometry
optimization using
the MM method

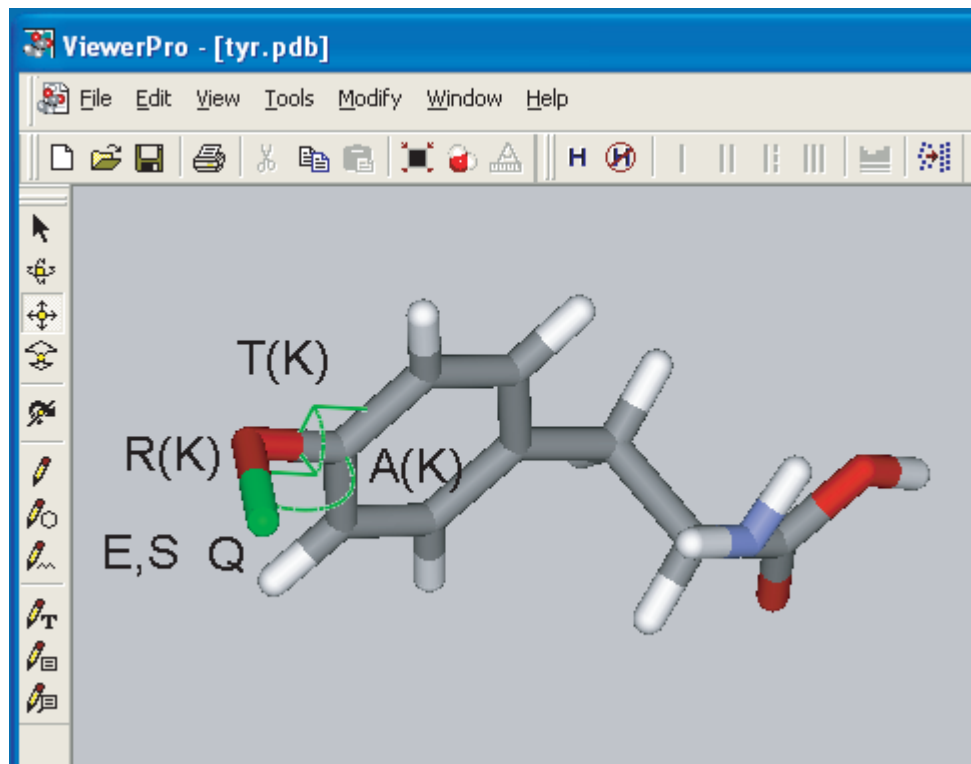
E and S
parameters for
Chlorine are
modified in order
to have the same
geometry of the
dimer as from the
QM calculations



MM parameters (Chloro-tyrosine)

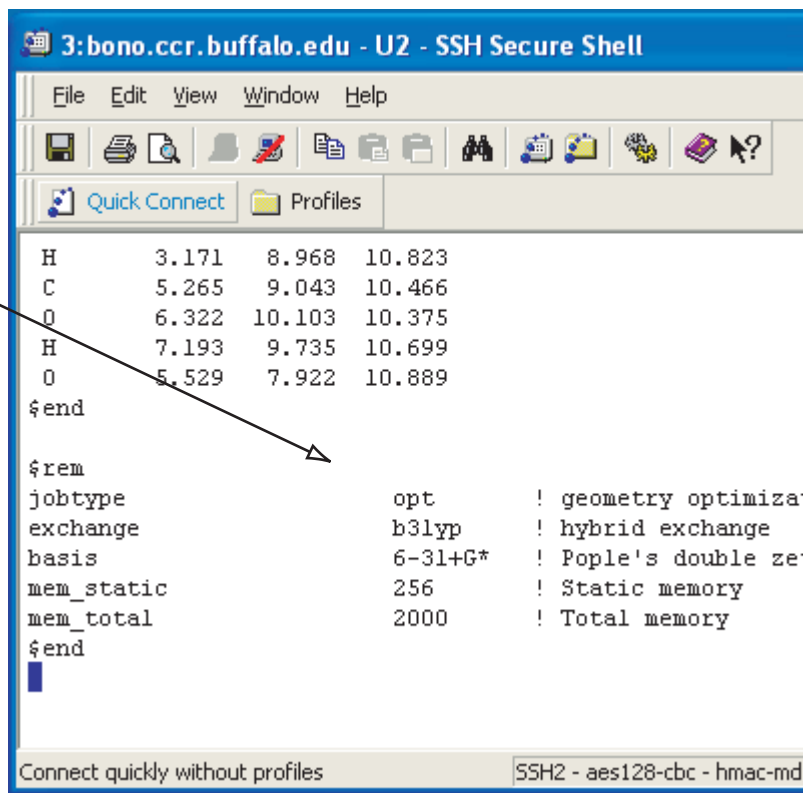
New atom

- Distance (Cons.)
- Angle (Const.)
- Torsion (Const.)
- Charge
- Van der Waals



MM parameters (Chloro-tyrosine)

QM geometry optimization of the molecule in the gas phase



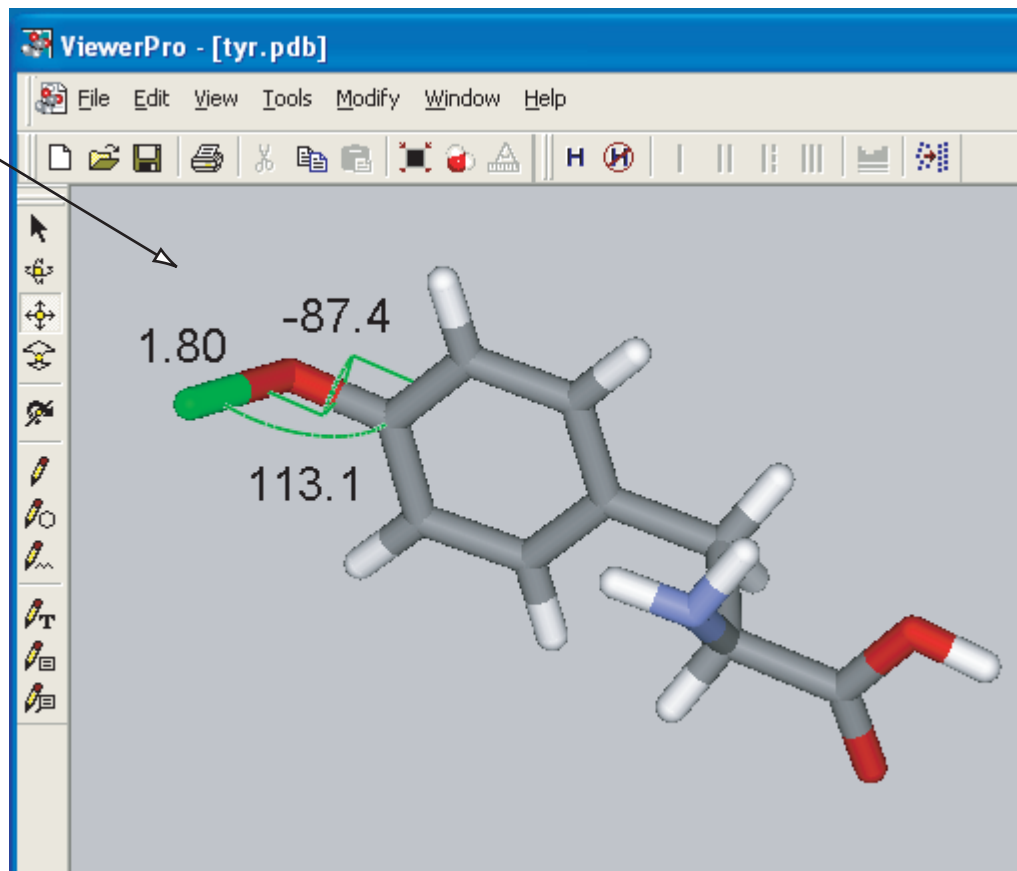
```
3:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
H      3.171    8.968   10.823
C      5.265    9.043   10.466
O      6.322   10.103   10.375
H      7.193    9.735   10.699
O      5.529    7.922   10.889
$end

$rem
jobtype                opt          ! geometry optimization
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double zeta
mem_static              256         ! Static memory
mem_total               2000        ! Total memory
$end
█

Connect quickly without profiles  SSH2 - aes128-cbc - hmac-md
```

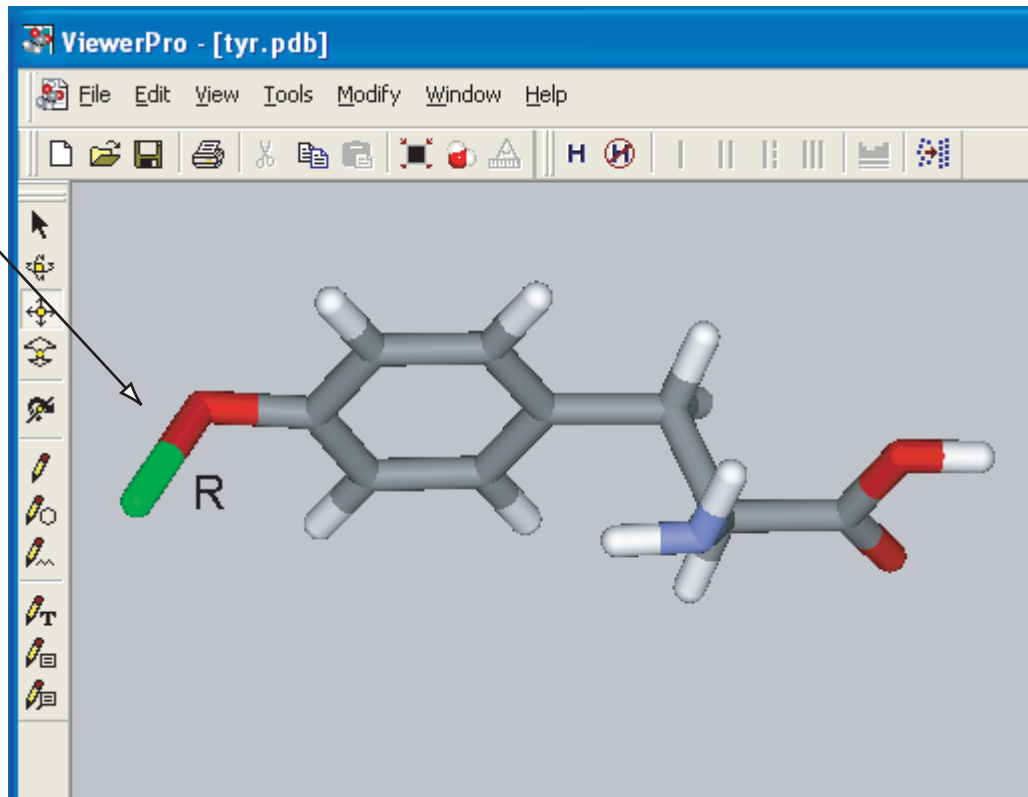

MM parameters (Chloro-tyrosine)

Results of the
calculations



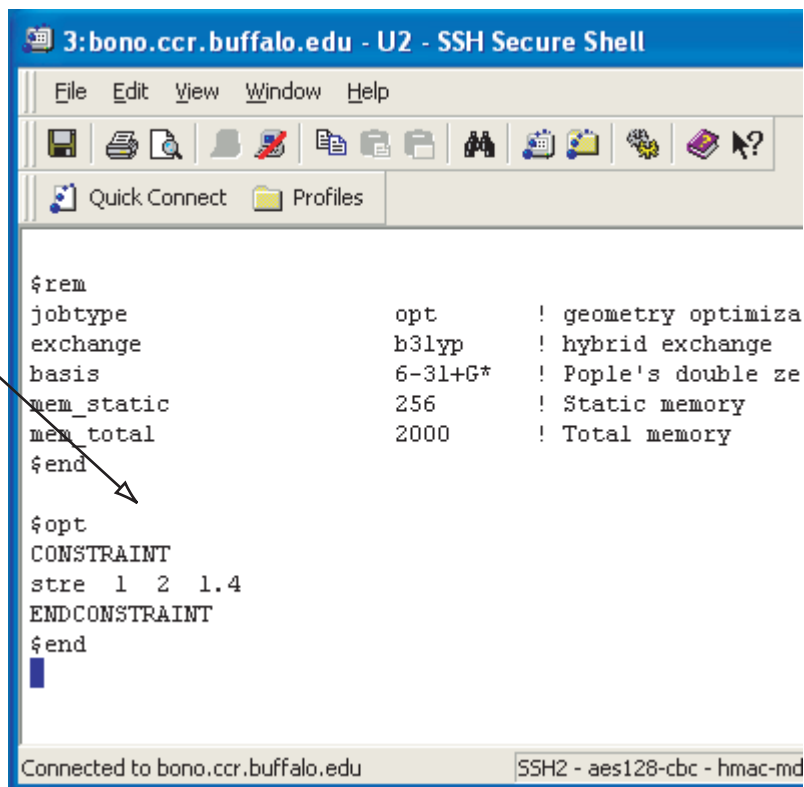
MM parameters (Chloro-tyrosine)

Calculations of the
optimal geometry
with a fixed
interatomic
distance



MM parameters (Chloro-tyrosine)

Constrained interatomic distance



```
3:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

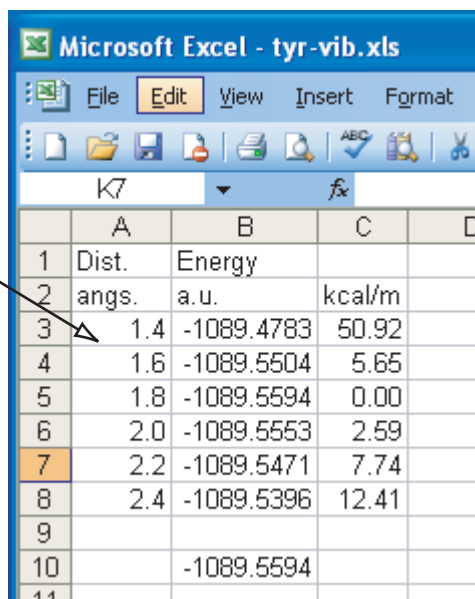
$rem
jobtype                opt          ! geometry optimiza
exchange               b3lyp        ! hybrid exchange
basis                  6-31+G*      ! Pople's double ze
mem_static             256          ! Static memory
mem_total              2000         ! Total memory
$end

$opt
CONSTRAINT
stre 1 2 1.4
ENDCONSTRAINT
$end
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md

MM parameters (Chloro-tyrosine)

Results of the
calculations



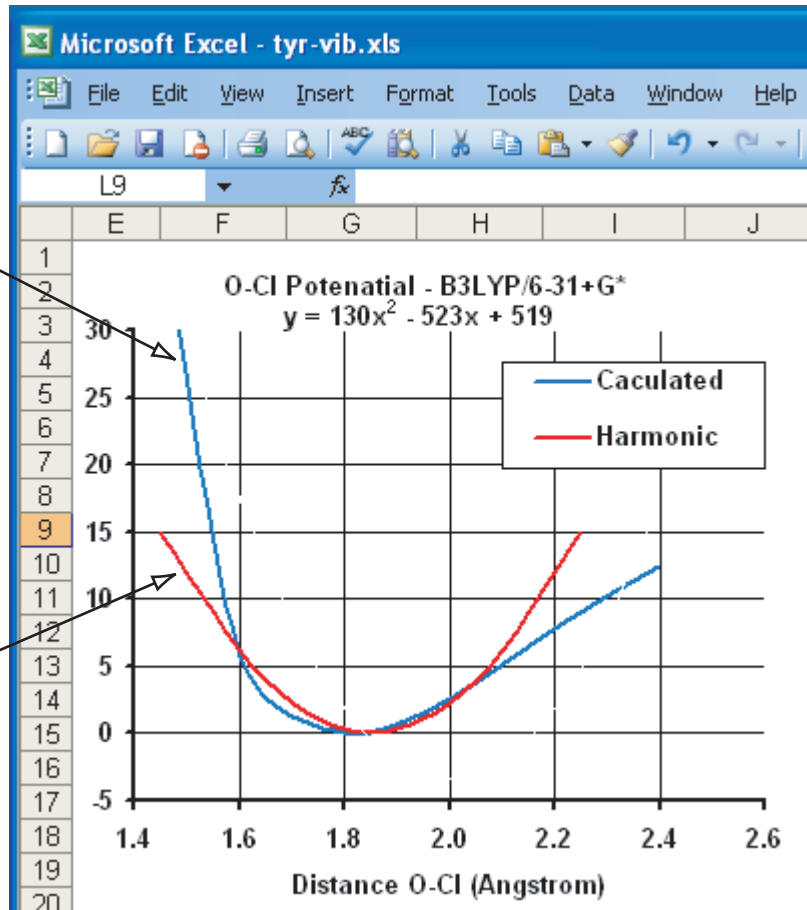
	A	B	C	D
1	Dist.	Energy		
2	angs.	a.u.	kcal/m	
3	1.4	-1089.4783	50.92	
4	1.6	-1089.5504	5.65	
5	1.8	-1089.5594	0.00	
6	2.0	-1089.5553	2.59	
7	2.2	-1089.5471	7.74	
8	2.4	-1089.5396	12.41	
9				
10		-1089.5594		
11				

MM parameters (Chloro-tyrosine)

Potential energy
surface of the O-Cl
stretching

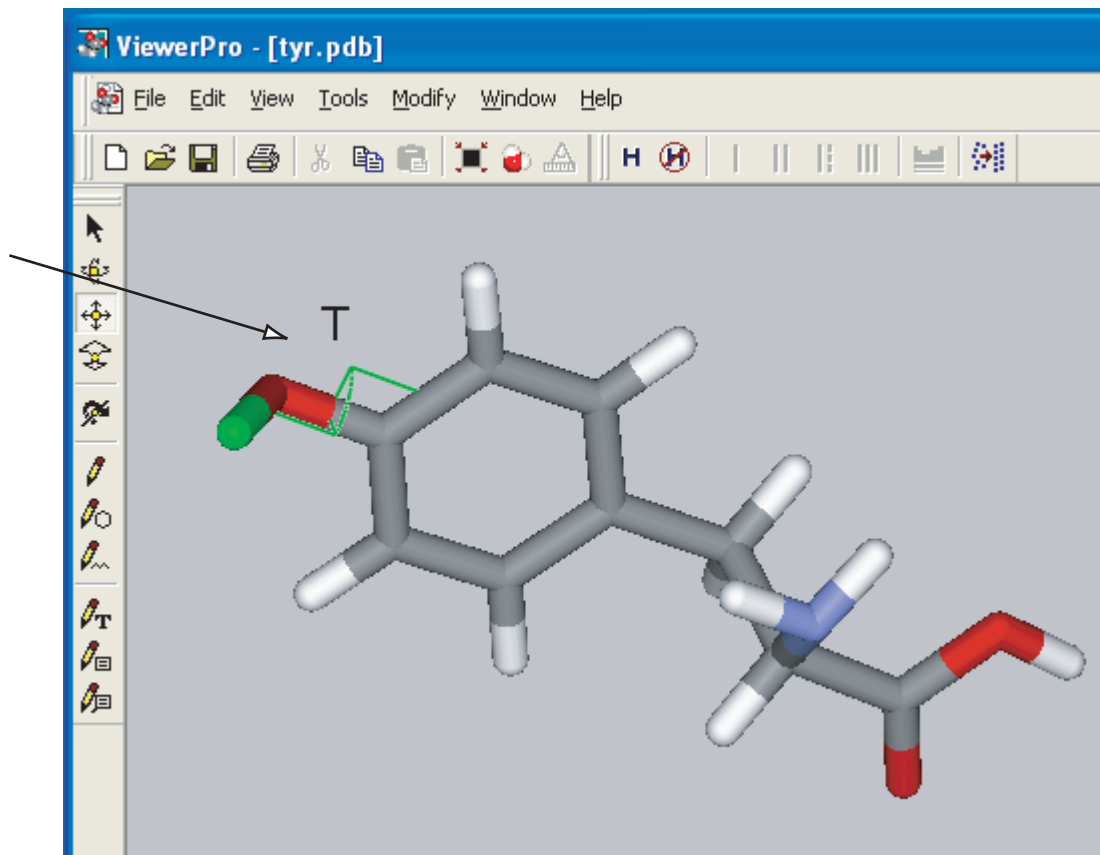
Harmonic
approximation:

$$E = \frac{1}{2} K (q - q_0)^2$$



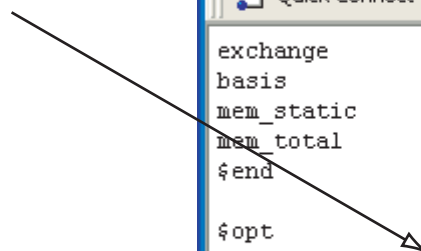
MM parameters (Chloro-tyrosine)

Geometry
optimization
with a
constrained
torsion angle



MM parameters (Chloro-tyrosine)

Geometry optimization
with a constrained torsion
angle



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

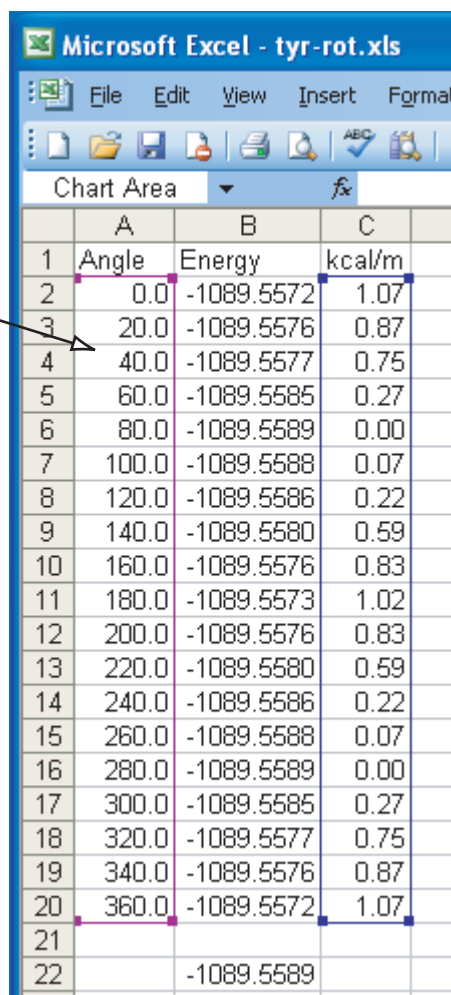
exchange          b3lyp      ! hybrid exchange
basis             6-31+G*   ! Pople's double zet
mem_static        256       ! Static memory
mem_total         2000      ! Total memory
$end

$opt
CONSTRAINT
tors 1 2 5 6 100.0
ENDCONSTRAINT
$end
█

Connected to bono.ccr.buffalo.edu      SSH2 - aes128-cbc - hmac-md5
```

MM parameters (Chloro-tyrosine)

Results of the
calculations

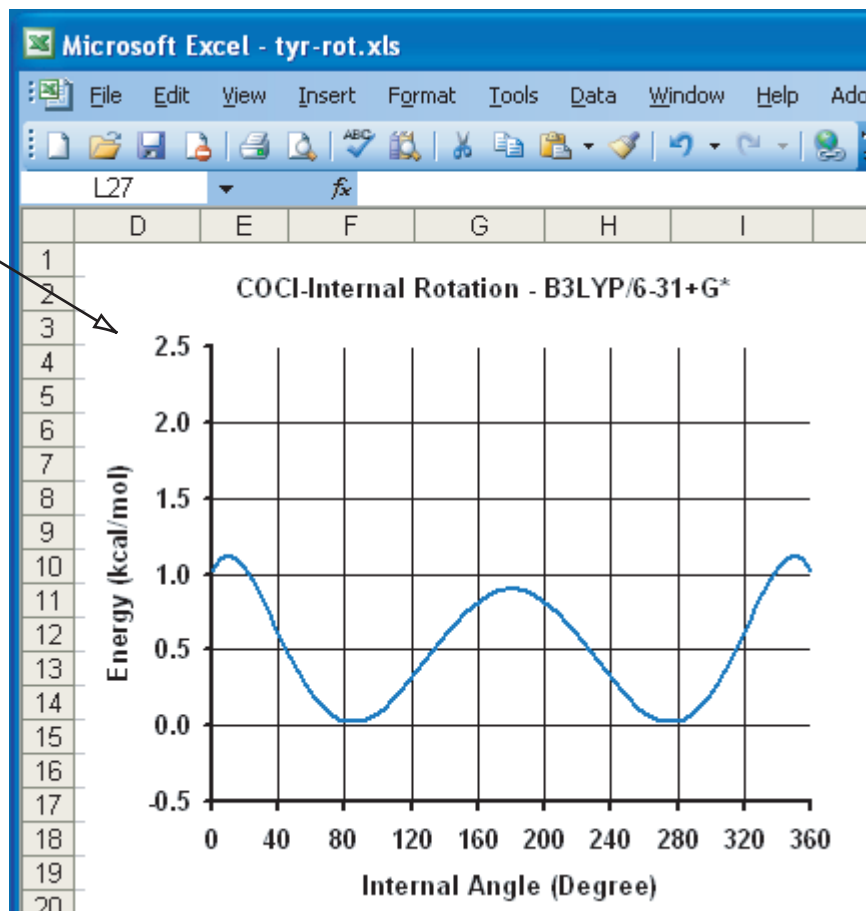


	A	B	C
1	Angle	Energy	kcal/m
2	0.0	-1089.5572	1.07
3	20.0	-1089.5576	0.87
4	40.0	-1089.5577	0.75
5	60.0	-1089.5585	0.27
6	80.0	-1089.5589	0.00
7	100.0	-1089.5588	0.07
8	120.0	-1089.5586	0.22
9	140.0	-1089.5580	0.59
10	160.0	-1089.5576	0.83
11	180.0	-1089.5573	1.02
12	200.0	-1089.5576	0.83
13	220.0	-1089.5580	0.59
14	240.0	-1089.5586	0.22
15	260.0	-1089.5588	0.07
16	280.0	-1089.5589	0.00
17	300.0	-1089.5585	0.27
18	320.0	-1089.5577	0.75
19	340.0	-1089.5576	0.87
20	360.0	-1089.5572	1.07
21			
22		-1089.5589	

MM parameters (Chloro-tyrosine)

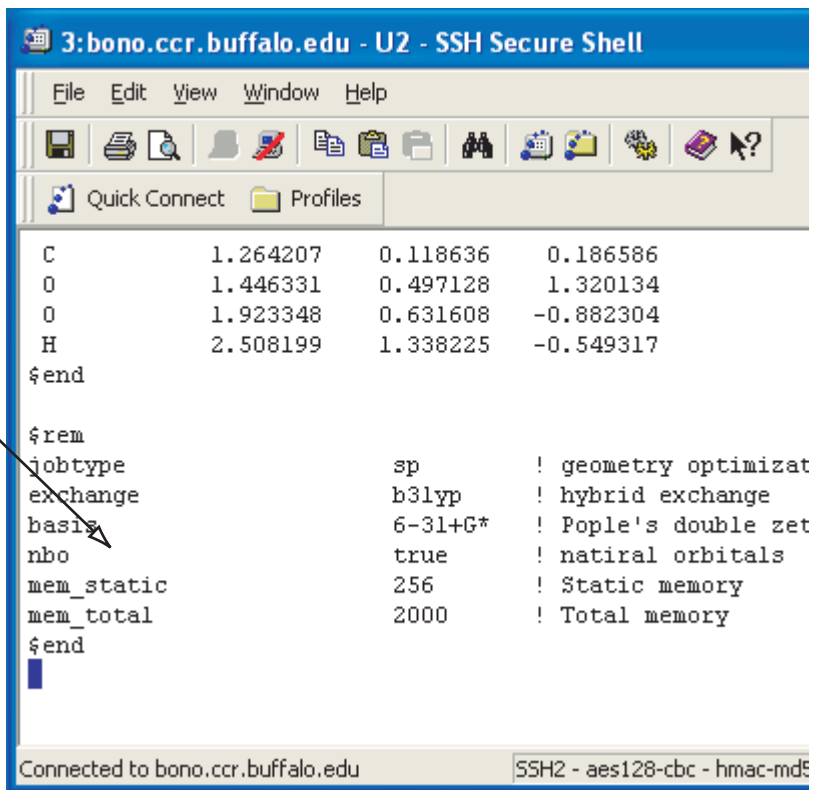
Potential energy surface of the internal rotation

- Angle at the minimum
- Energy at the maximum
- Number of maxima



MM parameters (Chloro-tyrosine)

Calculations of natural
orbitals



```
3:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
C      1.264207    0.118636    0.186586
O      1.446331    0.497128    1.320134
O      1.923348    0.631608   -0.882304
H      2.508199    1.338225   -0.549317
$end

$rem
jobtype          sp          ! geometry optimization
exchange         b3lyp        ! hybrid exchange
basis            6-31+G*      ! Pople's double zeta
nbo              true         ! natural orbitals
mem_static       256          ! Static memory
mem_total        2000         ! Total memory
$end
█


Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```



MM parameters (Chloro-tyrosine)

Atomic charges
calculated using
natural orbitals

1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell

FileEditViewWindowHelp



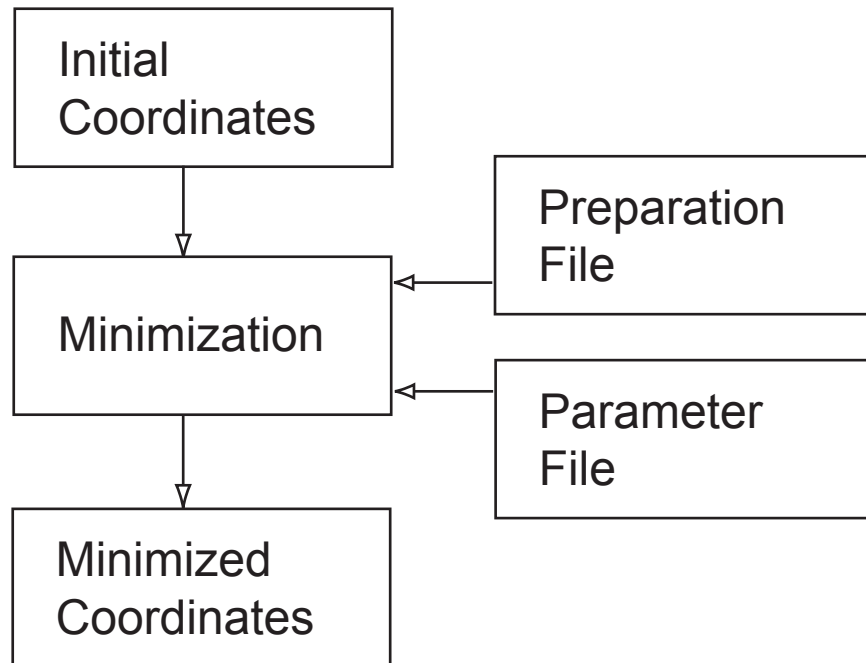
 Quick Connect Profiles

		Natural Charge	Natural Population		
Atom No			Core	Valence	Rydberg
C1	1	0.12906	9.99988	6.85690	0.01416
O	2	-0.48746	1.99975	6.46660	0.02111
C	3	0.27141	1.99879	3.70446	0.02534
C	4	-0.22947	1.99901	4.21371	0.01675
H	5	0.26086	0.00000	0.73793	0.00121
C	6	-0.23161	1.99904	4.21724	0.01533
H	7	0.24841	0.00000	0.75063	0.00096
C	8	-0.23122	1.99901	4.21550	0.01672
H	9	0.25980	0.00000	0.73899	0.00122
C	10	-0.23625	1.99905	4.22091	0.01628
H	11	0.24616	0.00000	0.75274	0.00110
C	12	-0.03054	1.99906	4.01377	0.01772

Connected to bono.ccr.buffalo.eduSSH2 - aes128-cbc - hmac-md5

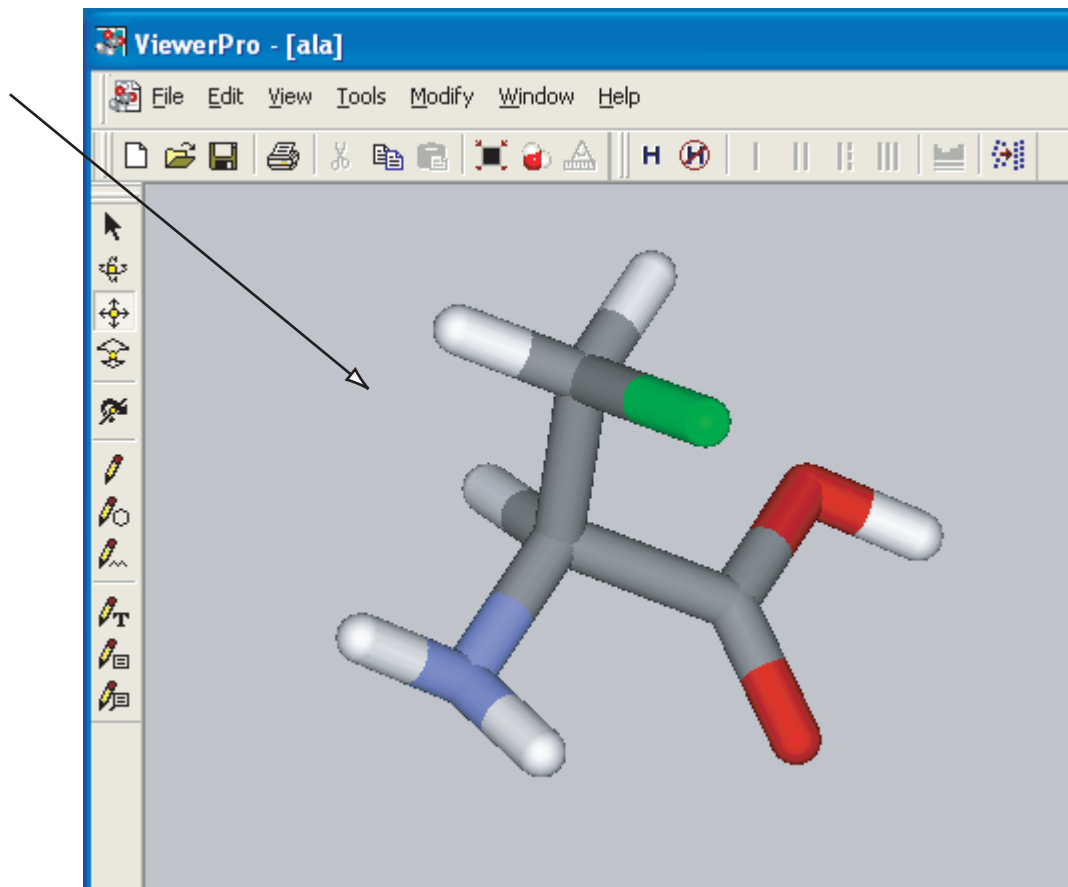
MM minimization of amino acids and base pairs

MM minimization requires two files: preparation and parameters files for each molecule (amino acid)



MM minimization of Chloro-alanine

Chloro-alanine



MM minimization of Chloro-alanine

Preparation file
of Chloro-
alanine

```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

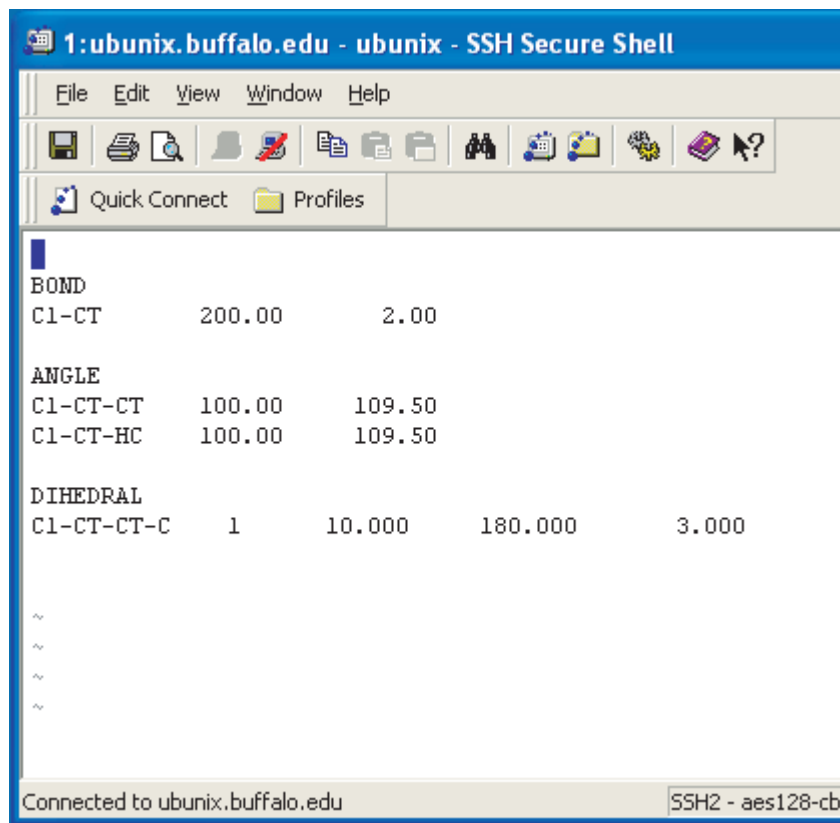
0 0 2

This is a remark line
molecule.res
ALT INT 0
CORRECT OMIT DU BEG
0.0000
1 DUMM DU M 0 -1 -2 0.000 .0 .0 .00000
2 DUMM DU M 1 0 -1 1.449 .0 .0 .00000
3 DUMM DU M 2 1 0 1.522 111.1 .0 .00000
4 CL C1 M 3 2 1 1.540 111.208 180.000 -0.17536
5 CB CT M 4 3 2 1.760 121.831 -142.502 -0.01283
6 HB2 H1 E 5 4 3 1.091 108.747 -21.473 0.09014
7 HB3 H1 E 5 4 3 1.090 109.844 -140.537 0.07698
8 CA CT M 5 4 3 1.521 110.198 98.150 0.12766
9 N N B 8 5 4 1.439 108.450 60.001 -0.89912
10 H H E 9 8 5 1.000 109.510 60.157 0.36630
11 HN H E 9 8 5 1.000 109.503 -59.804 0.37868
12 HA H1 E 8 5 4 1.092 109.251 -177.805 0.10168
13 C C M 8 5 4 1.512 111.755 -55.775 0.63173
14 O O E 13 8 5 1.234 119.824 76.845 -0.52787
"ala.in" 32L, 1318C

Connected to ubunix.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none
```

MM minimization of Chloro-alanine

Parameter file of Chloro-alanine



The screenshot shows an SSH terminal window titled "1: ubunix.buffalo.edu - ubunix - SSH Secure Shell". The window contains a parameter file for molecular minimization. The file lists bond lengths, angles, and dihedral angles for Chloro-alanine. The parameters are as follows:

BOND				
C1-CT	200.00	2.00		

ANGLE				
C1-CT-CT	100.00	109.50		
C1-CT-HC	100.00	109.50		

DIHEDRAL				
C1-CT-CT-C	1	10.000	180.000	3.000

Below the dihedral parameters, there are four tilde (~) characters. The terminal window also shows a status bar at the bottom indicating "Connected to ubunix.buffalo.edu" and "SSH2 - aes128-cb".

MM minimization of Chloro-alanine

Antechamber
program
generating the
preparation file
for Chloro-
alanine

```
#
[mfrein@bono ala]$ ls
ala.in      ala-mm.pdb      ANTECHAMBER_AC.ACO      ANTECHAMBER_PREP.A
ala-min.out ala.par          ANTECHAMBER_AM1BCC.AC   ATOMTYPE.INF
ala.min.out ala.pdb          ANTECHAMBER_AM1BCC_PRE.AC divcon.dmx
ala-min.pbs ala.top          ANTECHAMBER_BOND_TYPE.AC divcon.in
ala.min.pdb ala.xyz          ANTECHAMBER_BOND_TYPE.ACO divcon.out
ala.min.xyz ANTECHAMBER_AC.AC ANTECHAMBER_PREP.AC      divcon.rst
[mfrein@bono ala]$ module load amber/8
[mfrein@bono ala]$ ls
ala.in      ala-mm.pdb      ANTECHAMBER_AC.ACO      ANTECHAMBER_PREP.A
ala-min.out ala.par          ANTECHAMBER_AM1BCC.AC   ATOMTYPE.INF
ala.min.out ala.pdb          ANTECHAMBER_AM1BCC_PRE.AC divcon.dmx
ala-min.pbs ala.top          ANTECHAMBER_BOND_TYPE.AC divcon.in
ala.min.pdb ala.xyz          ANTECHAMBER_BOND_TYPE.ACO divcon.out
ala.min.xyz ANTECHAMBER_AC.AC ANTECHAMBER_PREP.AC      divcon.rst
[mfrein@bono ala]$ antechamber -i ala.pdb -fi pdb -o ala.in -fo prepi -c bcc
```

Connected to ubunix.buffalo.edu SSH2 - aes128cbc - hmac-md5 - none 98x1

PDB Input file

Prep output file

MM minimization of Chloro-alanine

Antechamber
program
generating the
preparation file
for Chloro-
alanine

```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_BOND_TYPE.ACO
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_BOND_TYPE.AC
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_AC.ACO
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_AC.AC
-rw-r--r-- 1 mfrein furlani 781 Dec 6 15:38 divcon.in
-rw-r--r-- 1 mfrein furlani 845 Dec 6 15:38 divcon.rst
-rw-r--r-- 1 mfrein furlani 16646 Dec 6 15:38 divcon.dmx
-rw-r--r-- 1 mfrein furlani 61394 Dec 6 15:38 divcon.out
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_AM1BCC_PRE.AC
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_AM1BCC.AC
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_PREP.ACO
-rw-r--r-- 1 mfrein furlani 1468 Dec 6 15:38 ANTECHAMBER_PREP.AC
-rw-r--r-- 1 mfrein furlani 3008 Dec 6 15:38 ATOMTYPE.INF
-rw-r--r-- 1 mfrein furlani 1318 Dec 6 15:38 ala.in
-rw-r--r-- 1 mfrein furlani 1557 Dec 6 15:38 PREP.INF
-rw-r--r-- 1 mfrein furlani 845 Dec 6 15:38 NEWPDB.PDB
[mfrein@bono ala]$
```

Connected to ubunix.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 98

New PDB file

MM minimization of Chloro-alanine

The preparation
file for Chloro-
alanine

```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

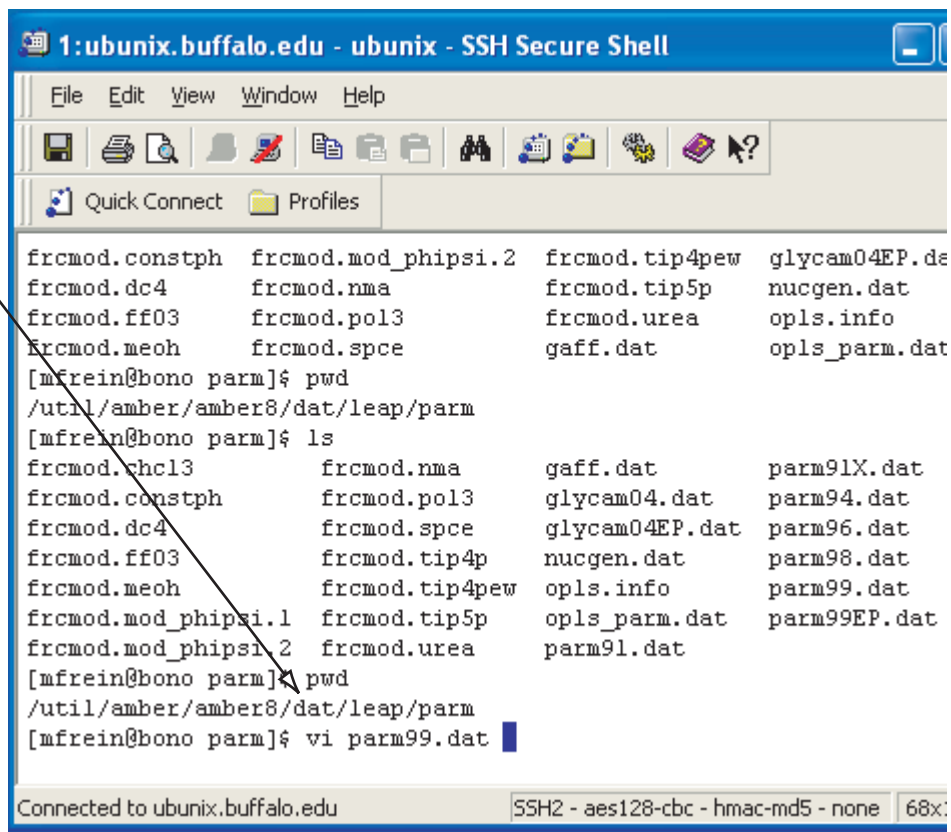
0 0 2

This is a remark line
molecule.res
ALT INT 0
CORRECT OMIT DU BEG
0.0000
1 DUMM DU M 0 -1 -2 0.000 .0 .0 .00000
2 DUMM DU M 1 0 -1 1.449 .0 .0 .00000
3 DUMM DU M 2 1 0 1.522 111.1 .0 .00000
4 CL c1 M 3 2 1 1.540 111.208 180.000 -0.17545
5 CB c3 M 4 3 2 1.760 121.831 -142.502 -0.01276
6 HB2 h1 E 5 4 3 1.091 108.747 -21.473 0.09003
7 HB3 h1 E 5 4 3 1.090 109.844 -140.537 0.07700
8 CA c3 M 5 4 3 1.521 110.198 98.150 0.12795
9 N n3 B 8 5 4 1.439 108.450 60.001 -0.89941
"ala.in" 32L 1318C
```

The atomic types should be corrected

MM minimization of Chloro-alanine

The home directory
of the AMBER
program

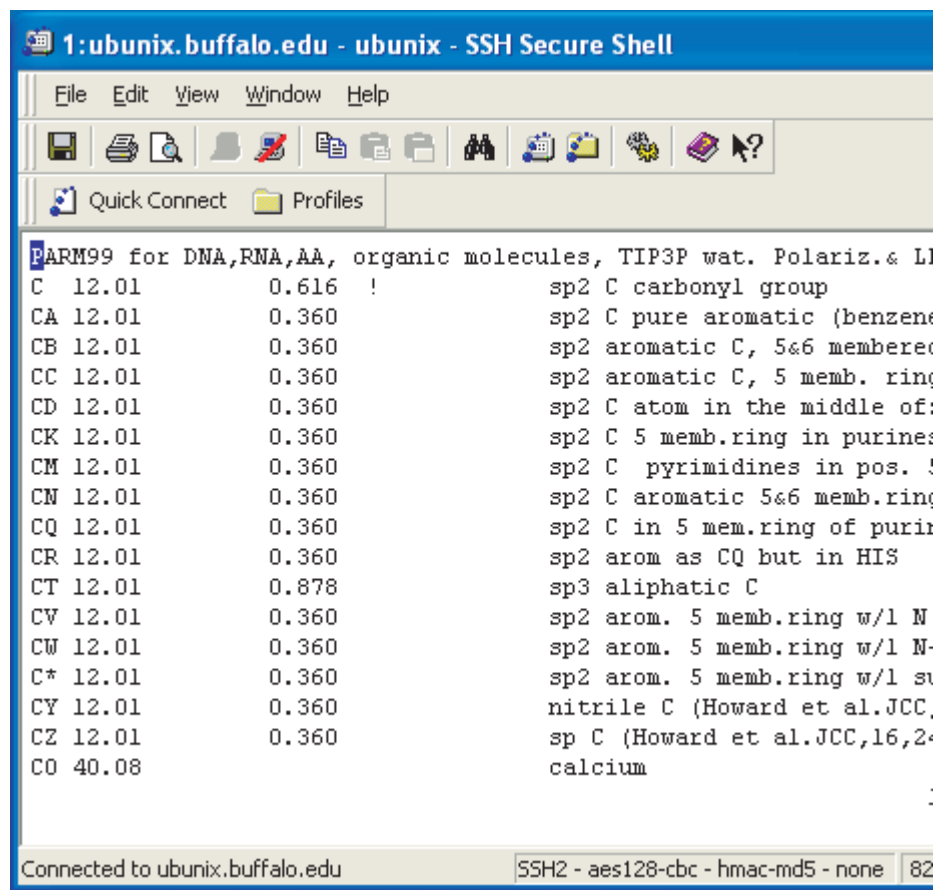


The screenshot shows an SSH terminal window titled "1:ubunix.buffalo.edu - ubunix - SSH Secure Shell". The terminal displays the output of the `pwd` and `ls` commands. The `pwd` command shows the current directory is `/util/amber/amber8/dat/leap/parm`. The `ls` command lists the contents of this directory, which are organized into four columns of files. A mouse cursor is visible over the `parm99.dat` file. The terminal window has a menu bar (File, Edit, View, Window, Help) and a toolbar with various icons. The status bar at the bottom indicates the connection is to `ubunix.buffalo.edu` using `SSH2 - aes128-cbc - hmac-md5 - none` with a resolution of `68x`.

```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
frcmod.constph frcmod.mod_hipsi.2 frcmod.tip4pew glycam04EP.da
frcmod.dc4 frcmod.nma frcmod.tip5p nucgen.dat
frcmod.ff03 frcmod.pol3 frcmod.urea opls.info
frcmod.meoh frcmod.spce gaff.dat opls_parm.dat
[mfrein@bono parm]$ pwd
/util/amber/amber8/dat/leap/parm
[mfrein@bono parm]$ ls
frcmod.chcl3 frcmod.nma gaff.dat parm91X.dat
frcmod.constph frcmod.pol3 glycam04.dat parm94.dat
frcmod.dc4 frcmod.spce glycam04EP.dat parm96.dat
frcmod.ff03 frcmod.tip4p nucgen.dat parm98.dat
frcmod.meoh frcmod.tip4pew opls.info parm99.dat
frcmod.mod_hipsi.1 frcmod.tip5p opls_parm.dat parm99EP.dat
frcmod.mod_hipsi.2 frcmod.urea parm91.dat
[mfrein@bono parm]$ pwd
/util/amber/amber8/dat/leap/parm
[mfrein@bono parm]$ vi parm99.dat
Connected to ubunix.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 68x
```

MM minimization of Chloro-alanine

The Parm99 file



The screenshot shows an SSH terminal window titled "1:ubunix.buffalo.edu - ubunix - SSH Secure Shell". The window has a menu bar (File, Edit, View, Window, Help) and a toolbar with various icons. Below the toolbar is a "Quick Connect" section with a "Profiles" button. The main text area displays the content of the Parm99 file, which is a table of parameters for different atom types. The table has three columns: atom type, a numerical value, and a description. The atom types listed are C, CA, CB, CC, CD, CK, CM, CN, CQ, CR, CT, CV, CW, C*, CY, CZ, and CO. The descriptions range from "sp2 C carbonyl group" to "calcium". The status bar at the bottom indicates "Connected to ubunix.buffalo.edu" and "SSH2 - aes128-cbc - hmac-md5 - none" with a session ID of 82.

```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

PARM99 for DNA,RNA,AA, organic molecules, TIP3P wat. Polariz.& LJ
C 12.01      0.616  !          sp2 C carbonyl group
CA 12.01      0.360          sp2 C pure aromatic (benzene
CB 12.01      0.360          sp2 aromatic C, 5&6 membere
CC 12.01      0.360          sp2 aromatic C, 5 memb. ring
CD 12.01      0.360          sp2 C atom in the middle of:
CK 12.01      0.360          sp2 C 5 memb.ring in purines
CM 12.01      0.360          sp2 C pyrimidines in pos. !
CN 12.01      0.360          sp2 C aromatic 5&6 memb.ring
CQ 12.01      0.360          sp2 C in 5 mem.ring of purin
CR 12.01      0.360          sp2 arom as CQ but in HIS
CT 12.01      0.878          sp3 aliphatic C
CV 12.01      0.360          sp2 arom. 5 memb.ring w/1 N
CW 12.01      0.360          sp2 arom. 5 memb.ring w/1 N-
C* 12.01      0.360          sp2 arom. 5 memb.ring w/1 su
CY 12.01      0.360          nitrile C (Howard et al.JCC,
CZ 12.01      0.360          sp C (Howard et al.JCC,16,2,
CO 40.08          calcium

Connected to ubunix.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none 82
```

MM minimization of Chloro-alanine

The parameter file for Chloro-alanine

Should be 1 for a particular torsion

The maximum energy divided by 2 and by number of torsions involved in this bond

Should be 0 if the Maximum is at 0 degree

Should be 180 if the Minimum is at 0 degree

Number of maxima

```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

BOND
C1-CT      200.00      1.80

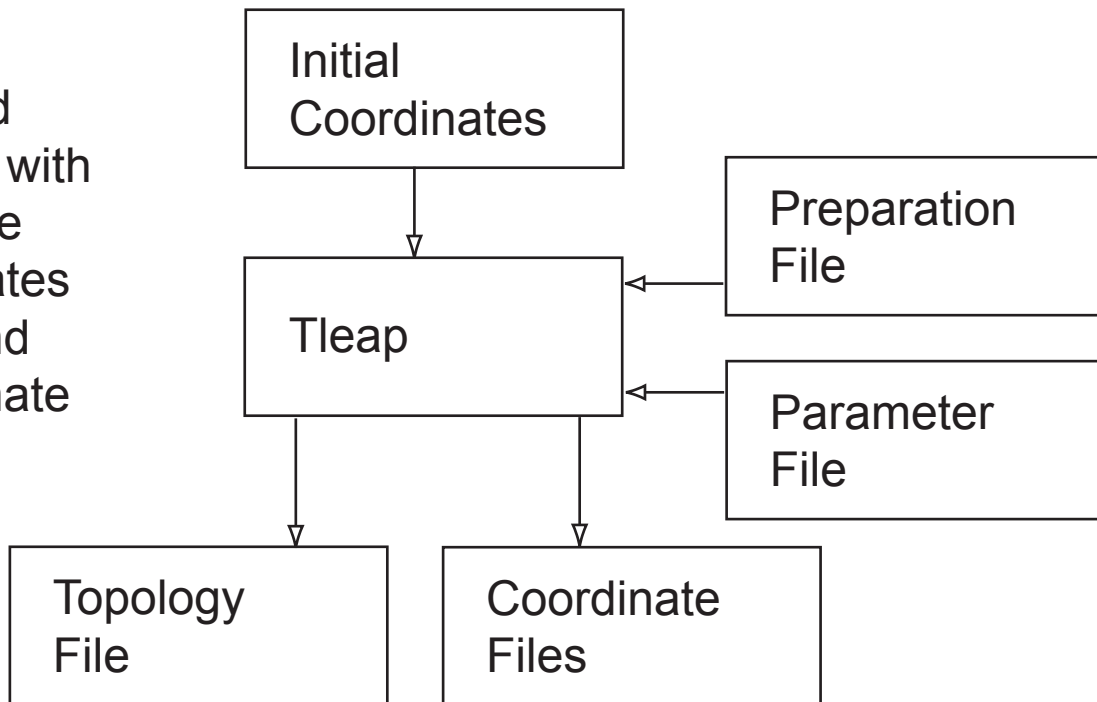
ANGLE
C1-CT-CT   100.00      113.00
C1-CT-HC   100.00      106.00

DIHEDRAL
C1-CT-CT-C 1      0.333      0.000      3.000
~
~
~
~
~
~

Connected to ubunix.buffalo.edu      SSH2 - aes128-cbc - hmac-md5 - nc
```

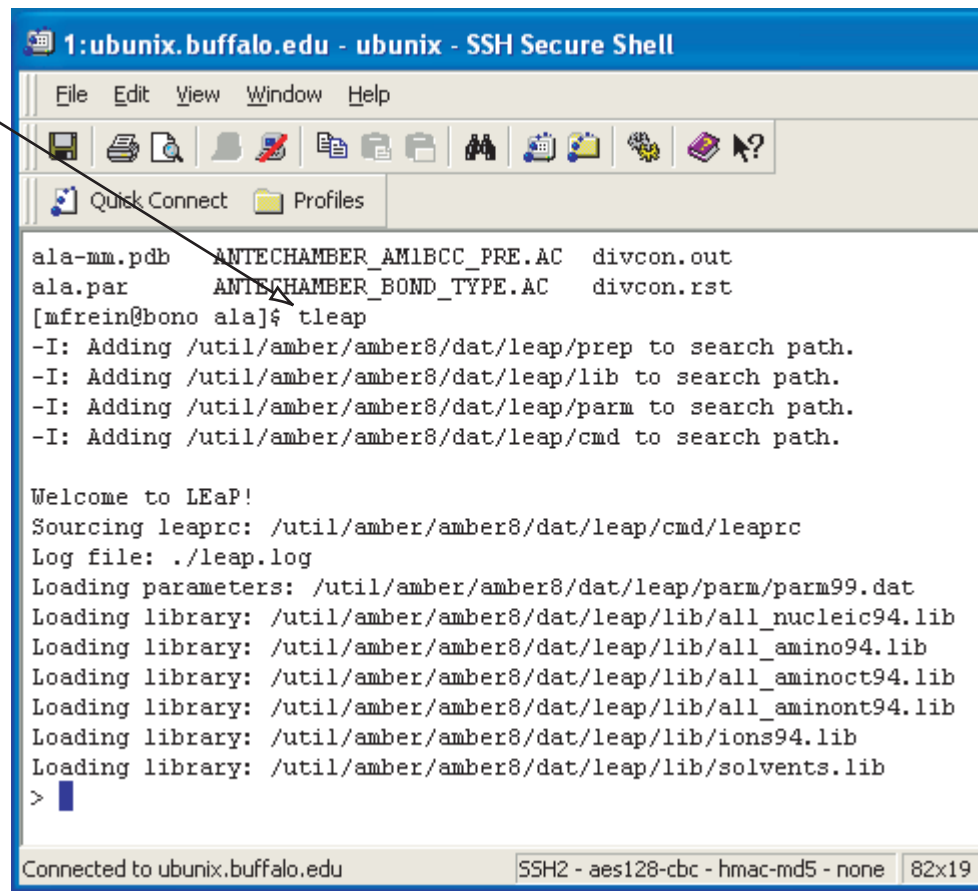
MM minimization of Chloro-alanine

Tleap program links the preparation and parameter files with initial coordinate file, and generates the topology and starting coordinate files



MM minimization of Chloro-alanine

Tleap program



```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Home, Back, Forward, Stop, Reload, Full Screen, Help]
Quick Connect Profiles

ala-mm.pdb ANTECHAMBER_AM1BCC_PRE.AC divcon.out
ala.par ANTECHAMBER_BOND_TYPE.AC divcon.rst
[mfrein@bono ala]$ tleap
-I: Adding /util/amber/amber8/dat/leap/prep to search path.
-I: Adding /util/amber/amber8/dat/leap/lib to search path.
-I: Adding /util/amber/amber8/dat/leap/parm to search path.
-I: Adding /util/amber/amber8/dat/leap/cmd to search path.

Welcome to LEaP!
Sourcing leaprc: /util/amber/amber8/dat/leap/cmd/leaprc
Log file: ./leap.log
Loading parameters: /util/amber/amber8/dat/leap/parm/parm99.dat
Loading library: /util/amber/amber8/dat/leap/lib/all_nucleic94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_amino94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminoc94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminont94.lib
Loading library: /util/amber/amber8/dat/leap/lib/ions94.lib
Loading library: /util/amber/amber8/dat/leap/lib/solvents.lib
>
```

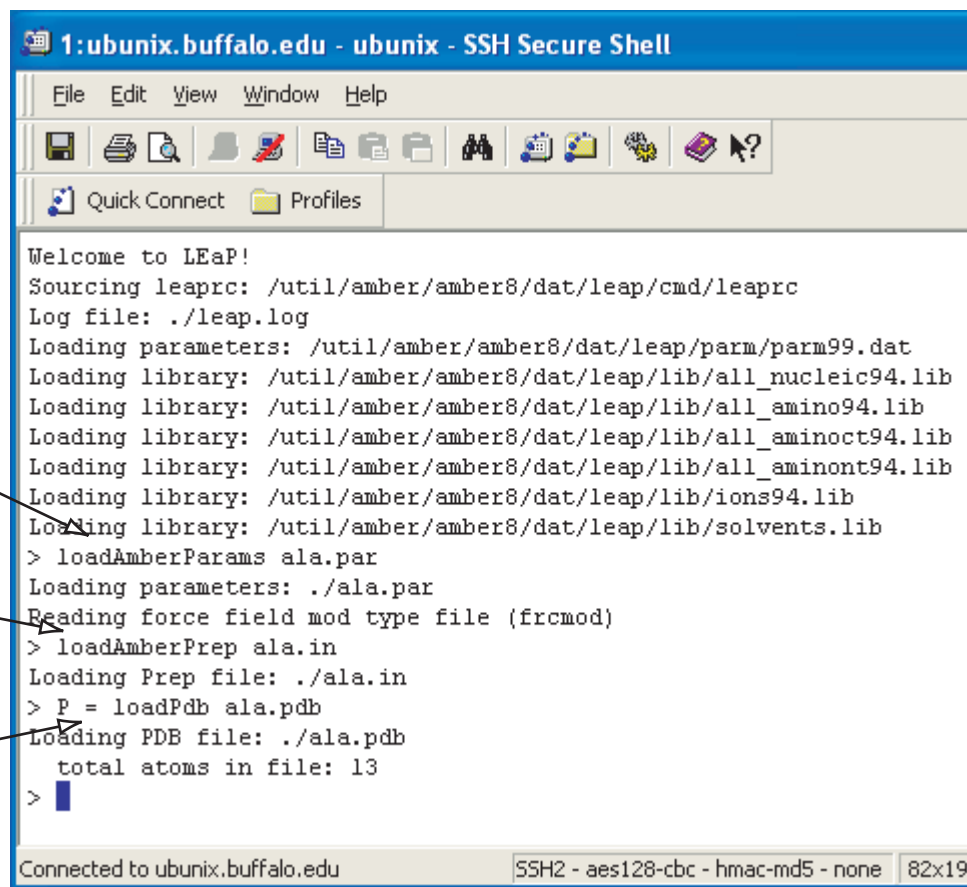
Connected to ubunix.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 82x19

MM minimization of Chloro-alanine

Loading
parameter file

Loading
preparation file

Loading
coordinate file

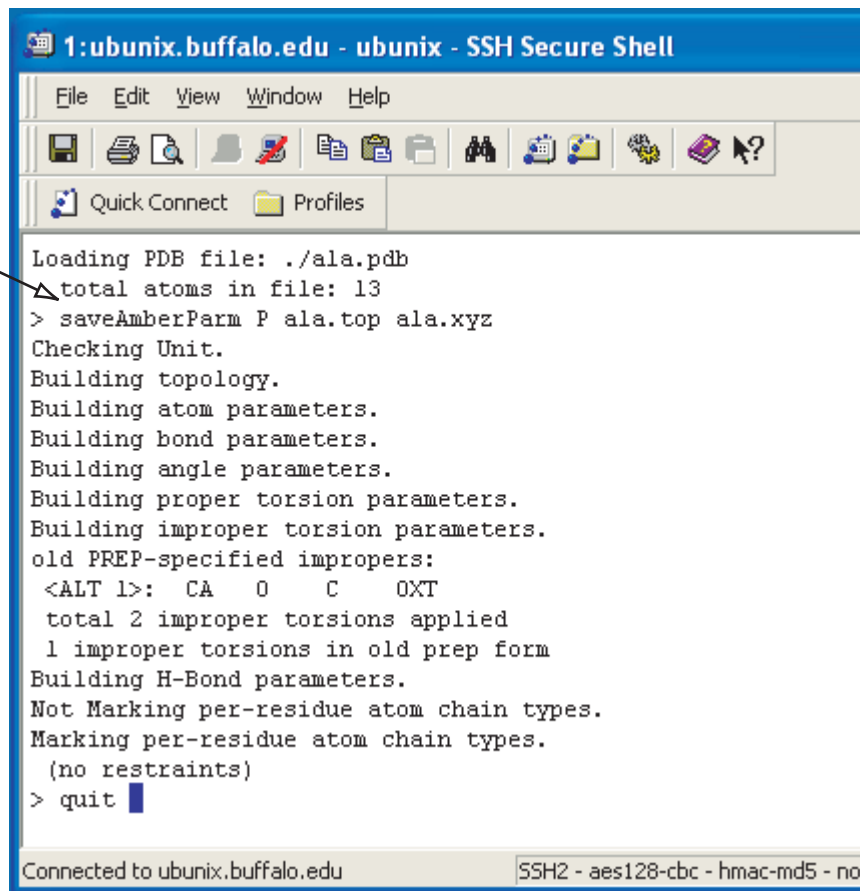


```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
Welcome to LEaP!
Sourcing leaprc: /util/amber/amber8/dat/leap/cmd/leaprc
Log file: ./leap.log
Loading parameters: /util/amber/amber8/dat/leap/parm/parm99.dat
Loading library: /util/amber/amber8/dat/leap/lib/all_nucleic94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_amino94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminoc94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminont94.lib
Loading library: /util/amber/amber8/dat/leap/lib/ions94.lib
Loading library: /util/amber/amber8/dat/leap/lib/solvents.lib
> loadAmberParams ala.par
Loading parameters: ./ala.par
Reading force field mod type file (frcmod)
> loadAmberPrep ala.in
Loading Prep file: ./ala.in
> P = loadPdb ala.pdb
Loading PDB file: ./ala.pdb
total atoms in file: 13
>
```

Connected to ubunix.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 82x19

MM minimization of Chloro-alanine

Generating and saving the topology and initial coordinate files



```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Open, Save, Home, Recent, Run, Stop, Refresh, Help]
Quick Connect Profiles

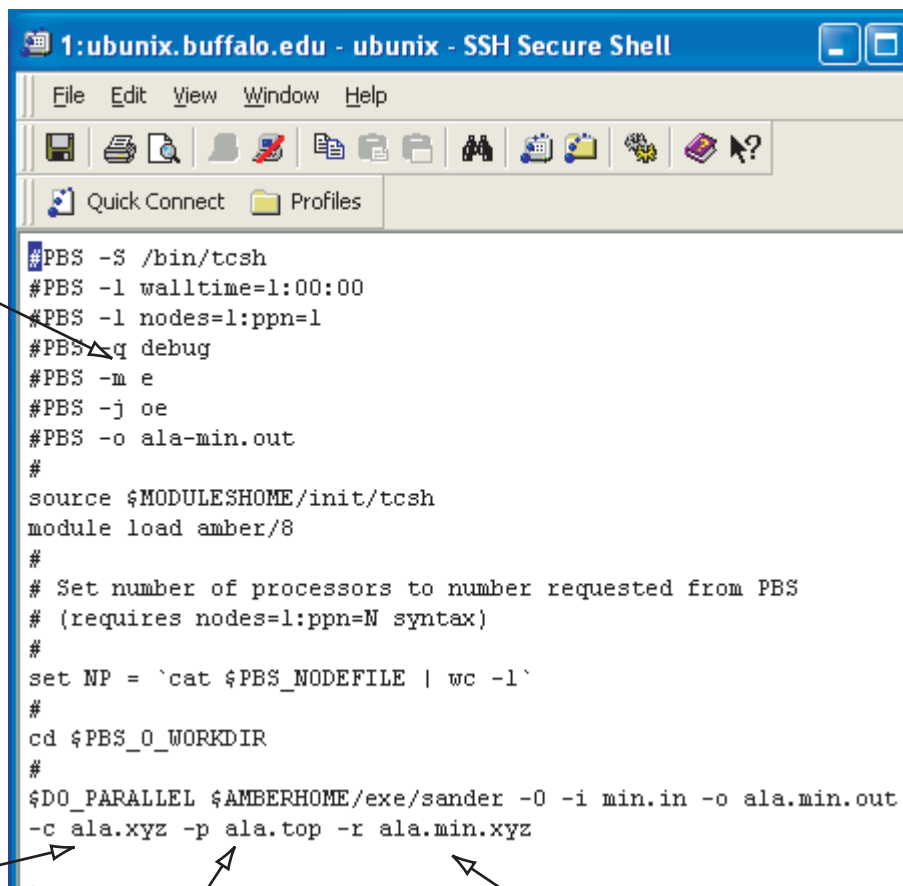
Loading PDB file: ./ala.pdb
^total atoms in file: 13
> saveAmberParm P ala.top ala.xyz
Checking Unit.
Building topology.
Building atom parameters.
Building bond parameters.
Building angle parameters.
Building proper torsion parameters.
Building improper torsion parameters.
old PREP-specified impropers:
<ALT 1>: CA  O  C  OXT
total 2 improper torsions applied
1 improper torsions in old prep form
Building H-Bond parameters.
Not Marking per-residue atom chain types.
Marking per-residue atom chain types.
(no restraints)
> quit
```

Connected to ubunix.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - no

Generating and saving by hand technical details of minimization

MM minimization of Chloro-alanine

Generating and saving by hand technical details of running the minimization



```
#PBS -S /bin/tcsh
#PBS -l walltime=1:00:00
#PBS -l nodes=1:ppn=1
#PBS -q debug
#PBS -m e
#PBS -j oe
#PBS -o ala-min.out
#
source $MODULESHOME/init/tcsh
module load amber/8
#
# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i min.in -o ala.min.out
-c ala.xyz -p ala.top -r ala.min.xyz
```

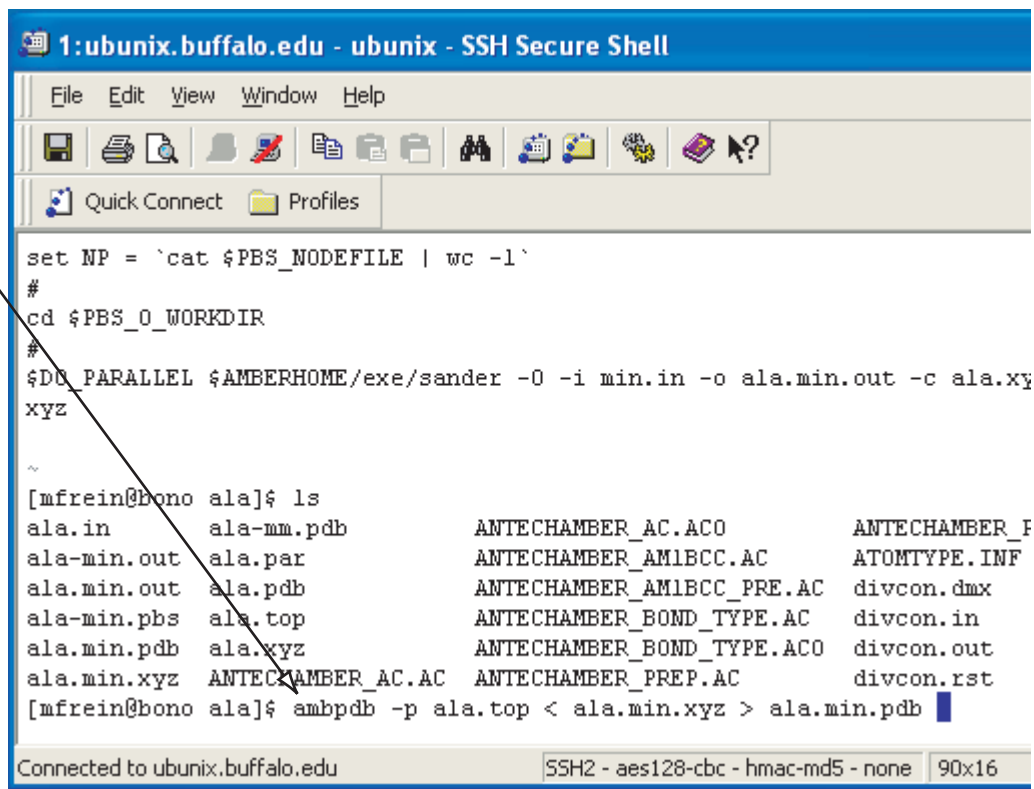
Initial coordinate file

Topology file

Minimized coordinate file

MM minimization of Chloro-alanine

Transforming the
coordinate file
into a PDB file



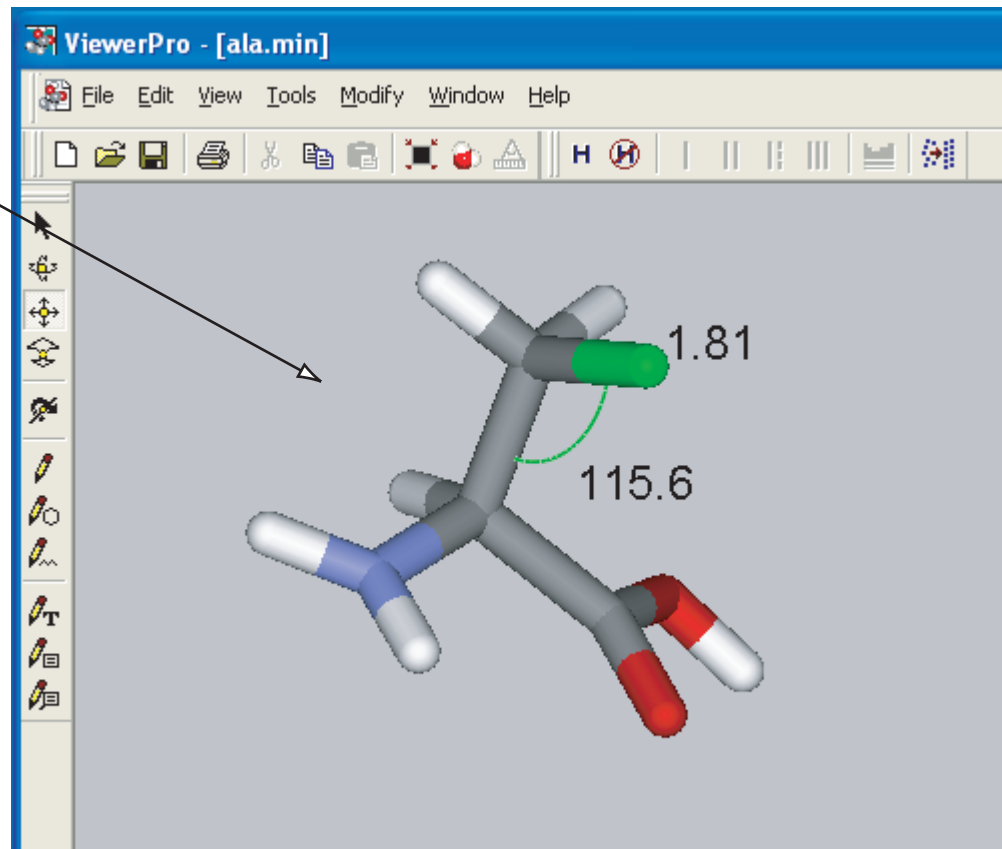
The screenshot shows an SSH terminal window titled "1:ubunix.buffalo.edu - ubunix - SSH Secure Shell". The terminal displays the following commands and output:

```
set NP = `cat $PBS_NODEFILE | wc -l`  
#  
cd $PBS_O_WORKDIR  
#  
$DO_PARALLEL $AMBERHOME/exe/sander -O -i min.in -o ala.min.out -c ala.xyz  
xyz  
~  
[mfrein@bono ala]$ ls  
ala.in      ala-mm.pdb      ANTECHAMBER_AC.ACO      ANTECHAMBER_F  
ala-min.out ala.par          ANTECHAMBER_AM1BCC.AC   ATOMTYPE.INF  
ala.min.out ala.pdb          ANTECHAMBER_AM1BCC_PRE.AC divcon.dmx  
ala-min.pbs ala.top          ANTECHAMBER_BOND_TYPE.AC divcon.in  
ala.min.pdb ala.xyz          ANTECHAMBER_BOND_TYPE.ACO divcon.out  
ala.min.xyz ANTECHAMBER_AC.AC ANTECHAMBER_PREP.AC      divcon.rst  
[mfrein@bono ala]$ ambpdb -p ala.top < ala.min.xyz > ala.min.pdb
```

The terminal window also shows a menu bar with "File", "Edit", "View", "Window", and "Help". Below the menu bar is a toolbar with various icons. At the bottom of the window, it says "Connected to ubunix.buffalo.edu" and "SSH2 - aes128-cbc - hmac-md5 - none 90x16".

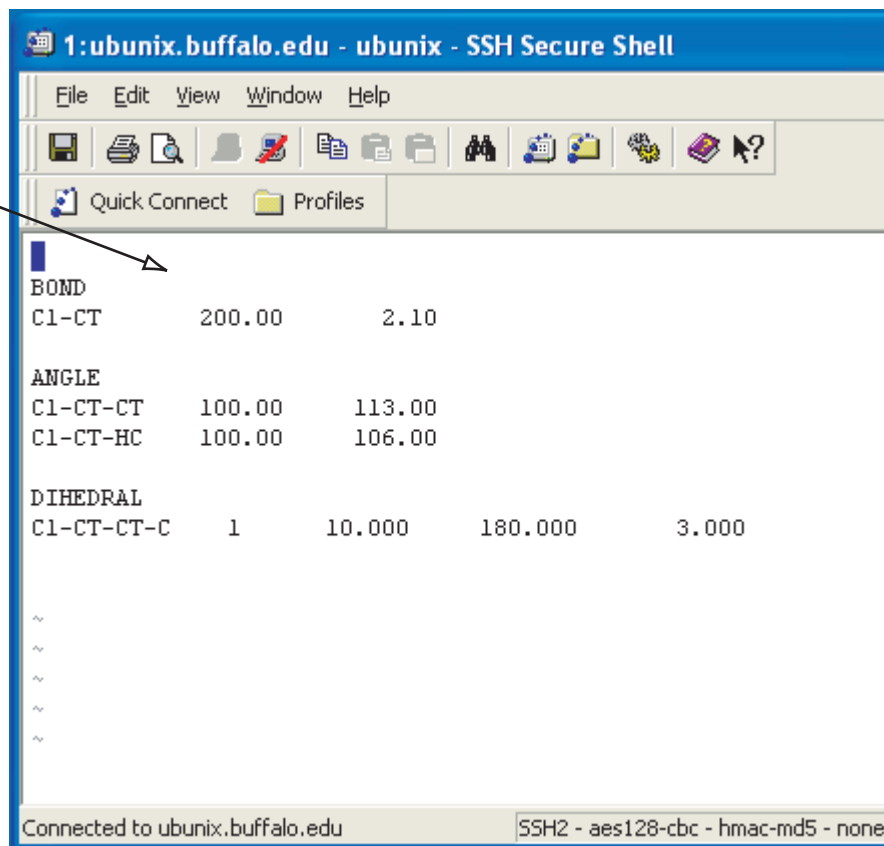
MM minimization of Chloro-alanine

Optimal geometry
of Chloro-alanine
after MM
minimization



MM minimization of Chloro-alanine

Modified
parameter file of
Chloro-alanine



```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Open, Save, Run, Stop, Help]
Quick Connect Profiles

BOND
C1-CT      200.00      2.10

ANGLE
C1-CT-CT   100.00      113.00
C1-CT-HC   100.00      106.00

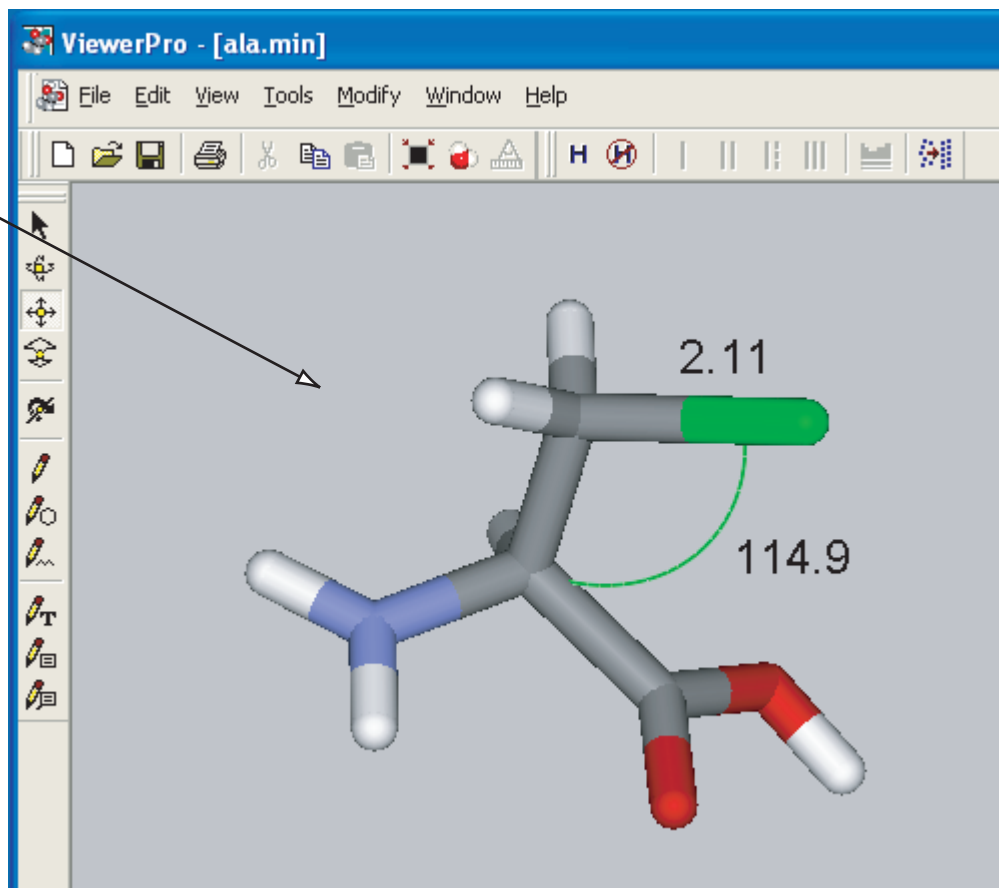
DIHEDRAL
C1-CT-CT-C 1      10.000     180.000     3.000

~
~
~
~
~

Connected to ubunix.buffalo.edu      SSH2 - aes128-cbc - hmac-md5 - none
```

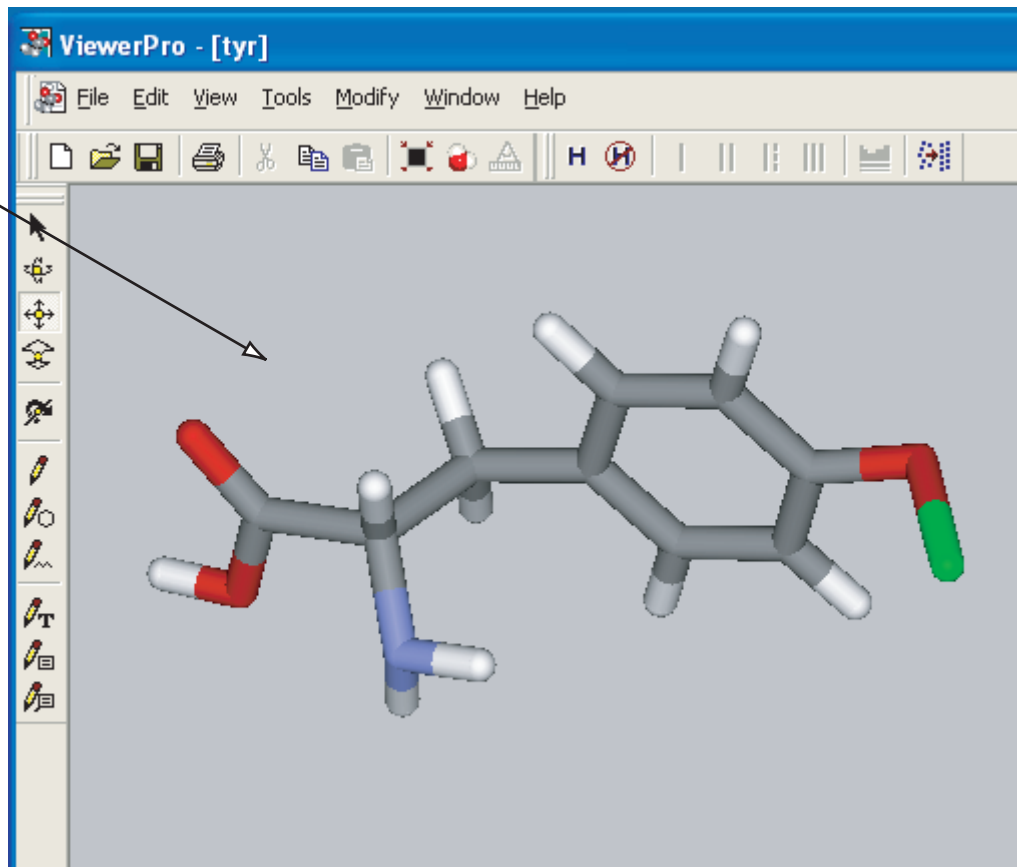
MM minimization of Chloro-alanine

Optimal structure
of Chloro-alanine
after parameter
modification



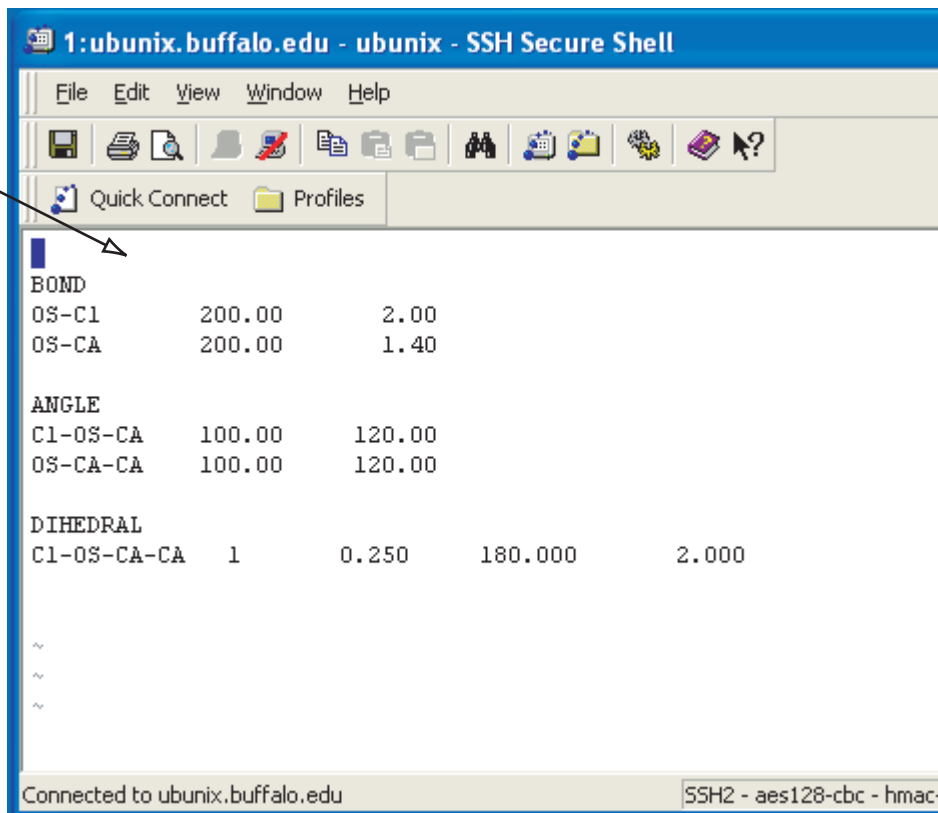
MM minimization of Chloro-tyrosine

Optimal structure
of Chloro-tyrosine
after QM
calculations



MM minimization of Chloro-tyrosine

The parameter
file of Chloro-
tyrosine



```
1:ubunix.buffalo.edu - ubunix - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

BOND
OS-C1      200.00      2.00
OS-CA      200.00      1.40

ANGLE
C1-OS-CA   100.00      120.00
OS-CA-CA   100.00      120.00

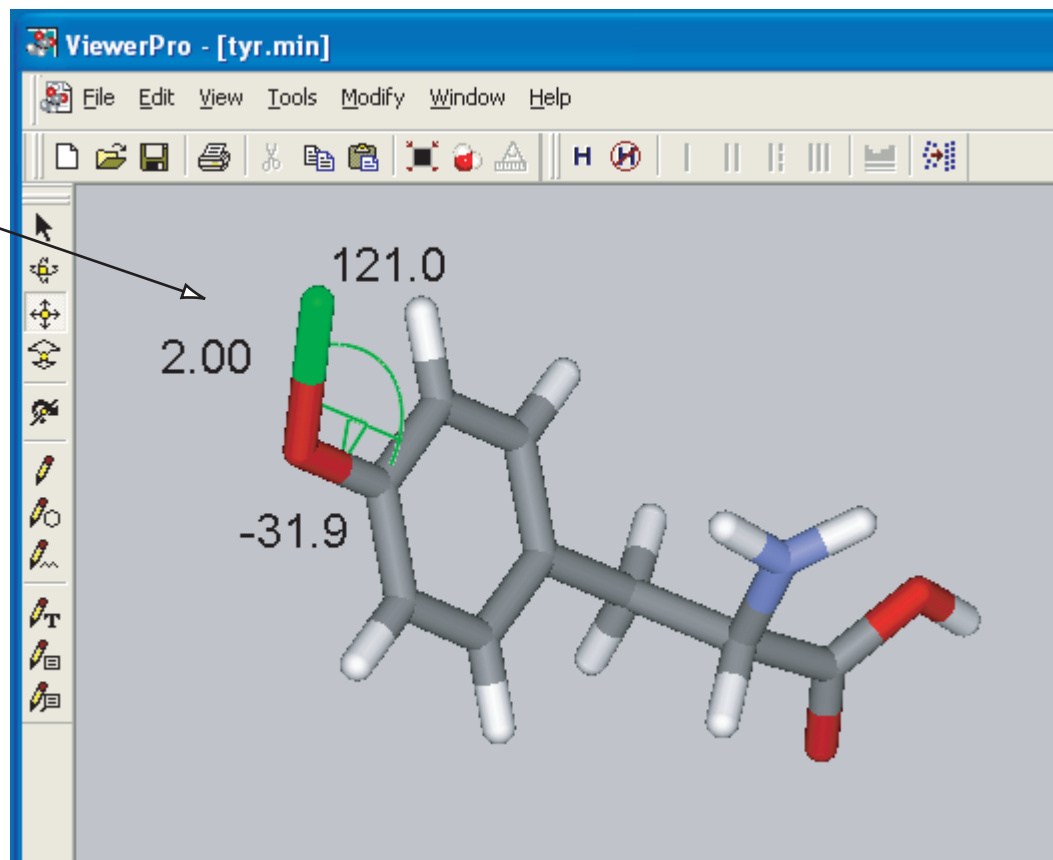
DIHEDRAL
C1-OS-CA-CA 1      0.250      180.000      2.000

~
~
~

Connected to ubunix.buffalo.edu      SSH2 - aes128-cbc - hmac
```

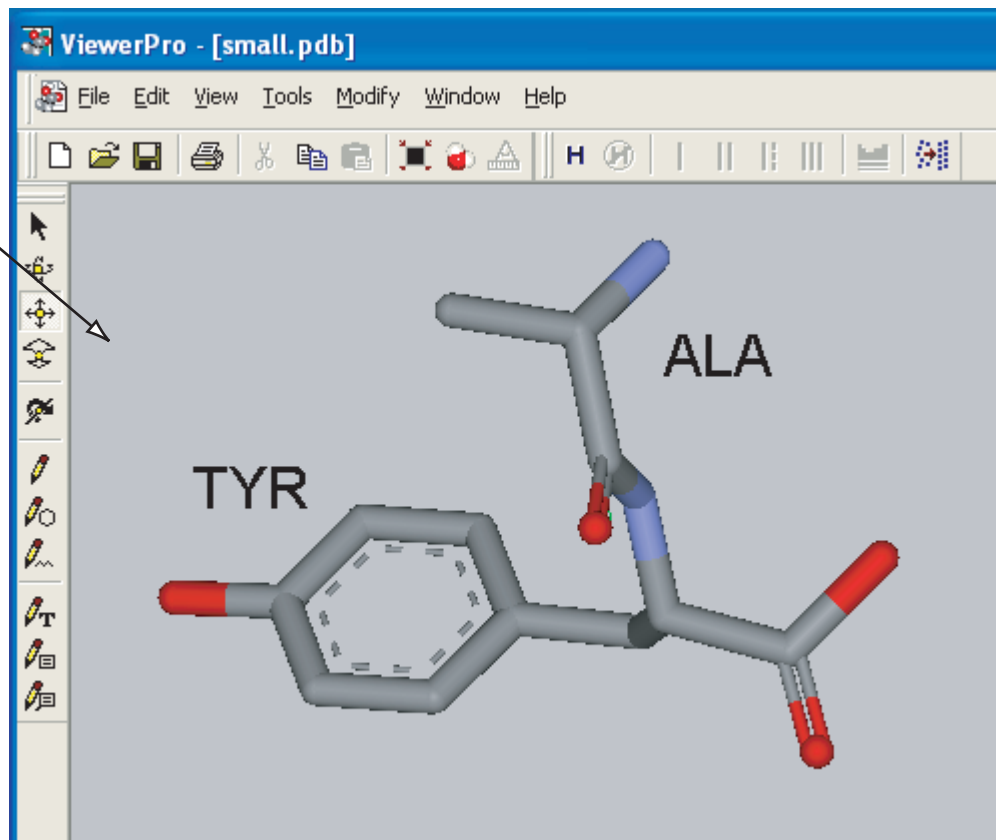
MM minimization of Chloro-tyrosine

The optimal geometry of Chloro-tyrosine after modified MM minimization



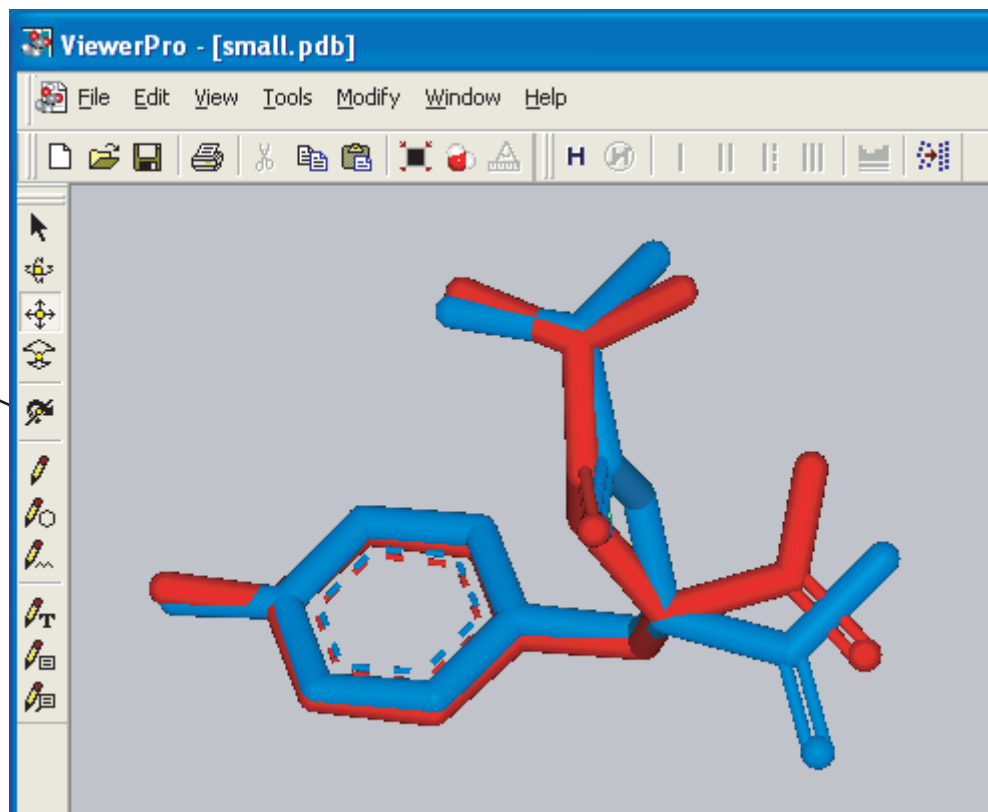
MM minimization of a small peptide

The initial
geometry of
ALA-TYR
peptide



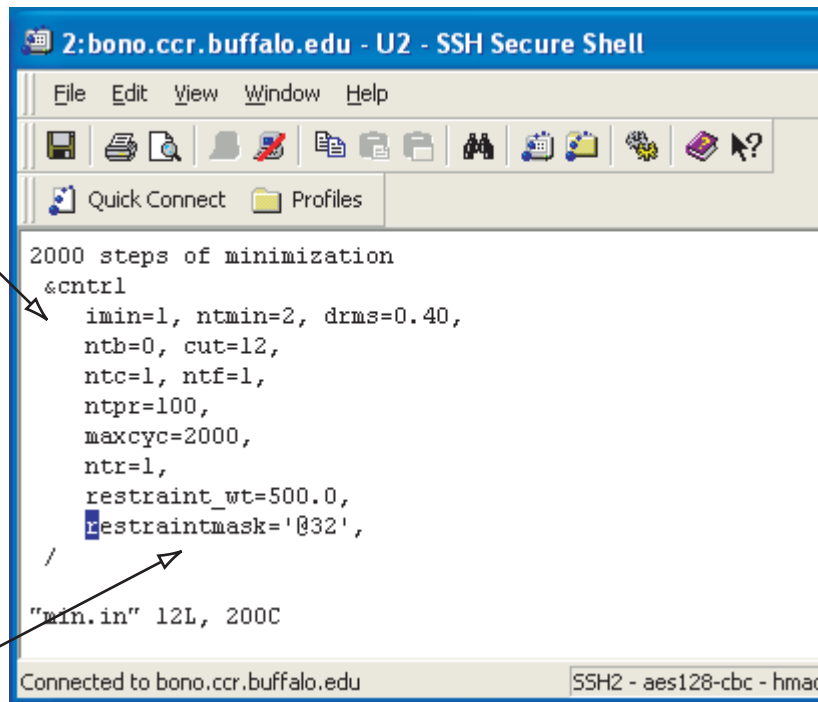
MM minimization of a small peptide

The minimized structure of the peptide (red) compared with the initial structure of this molecule (blue)



MM minimization of a small peptide

The input file of minimization with absolute constrains



```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

2000 steps of minimization
&cntrl
  imin=1, ntmin=2, drms=0.40,
  ntb=0, cut=12,
  ntc=1, ntf=1,
  ntp=100,
  maxcyc=2000,
  ntr=1,
  restraint_wt=500.0,
  restraintmask='@32',
/

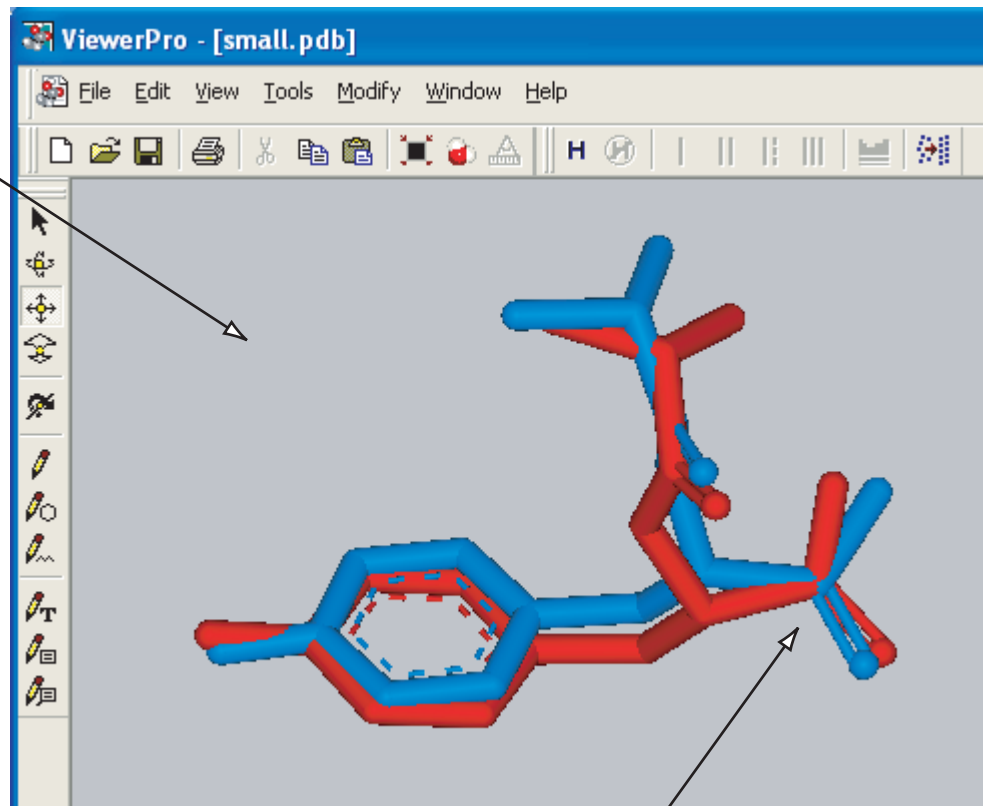
"min.in" 12L, 200C

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac
```

The position of the atom 32 is constrained

MM minimization of a small peptide

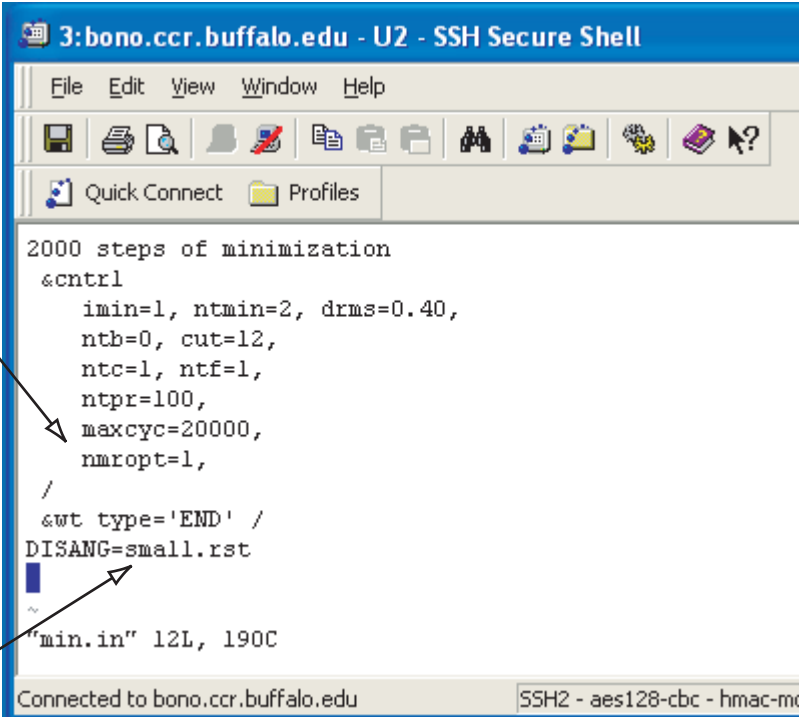
The initial (blue) and final (red) geometry of the peptide after minimization with a constrained position of the carbon atom



The constrained atom

MM minimization of a small peptide

The input file of minimization with relative constrains



The screenshot shows an SSH terminal window titled "3: bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The terminal displays the following commands and output:

```
2000 steps of minimization
&cntrl
    imin=1, ntmin=2, drms=0.40,
    ntb=0, cut=12,
    ntc=1, ntf=1,
    ntp=100,
    maxcyc=20000,
    nmropt=1,
/
&wt type='END' /
DISANG=small.rst
~
"min.in" 12L, 190C
```

At the bottom of the terminal, it shows "Connected to bono.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-mc".

The file with constrains

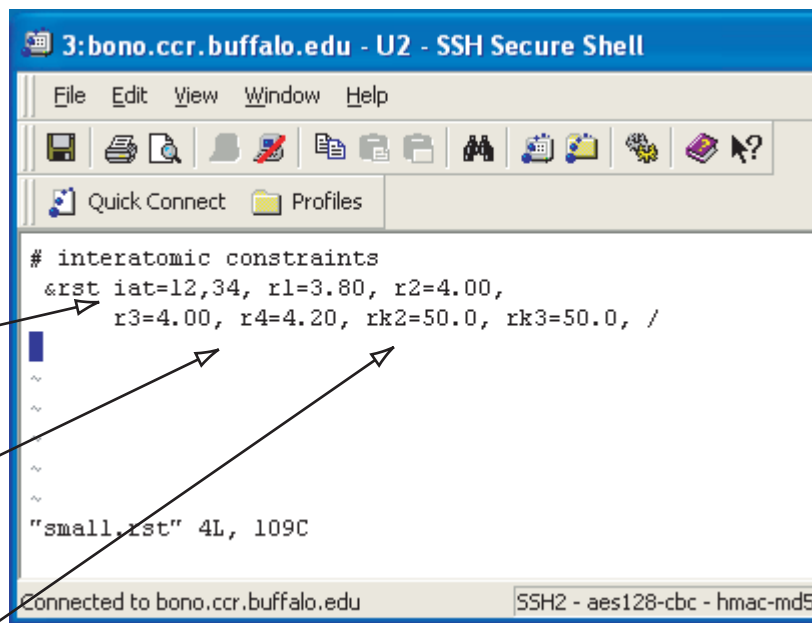
MM minimization of a small peptide

The constrains file

The atoms to be
constrained

The shape of
the potential

The potential
force constants

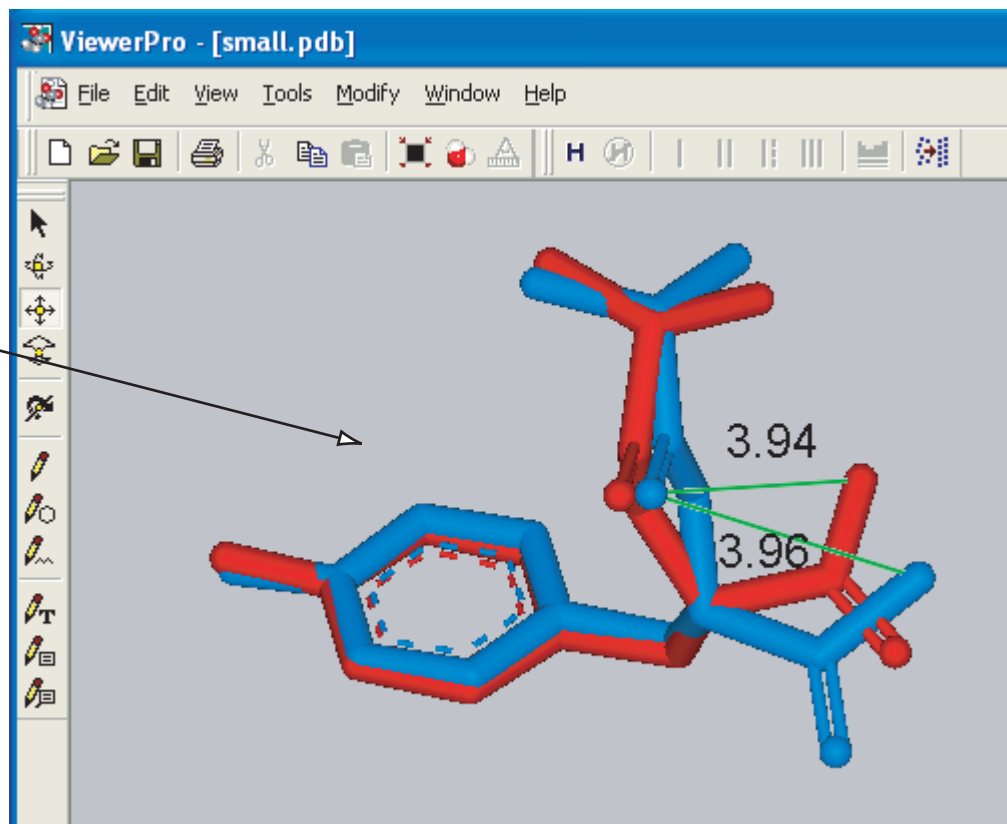


```
# interatomic constraints
&rst iat=12,34, r1=3.80, r2=4.00,
r3=4.00, r4=4.20, rk2=50.0, rk3=50.0, /

~
~
~
~
"small.rst" 4L, 109C
```


MM minimization of a small peptide

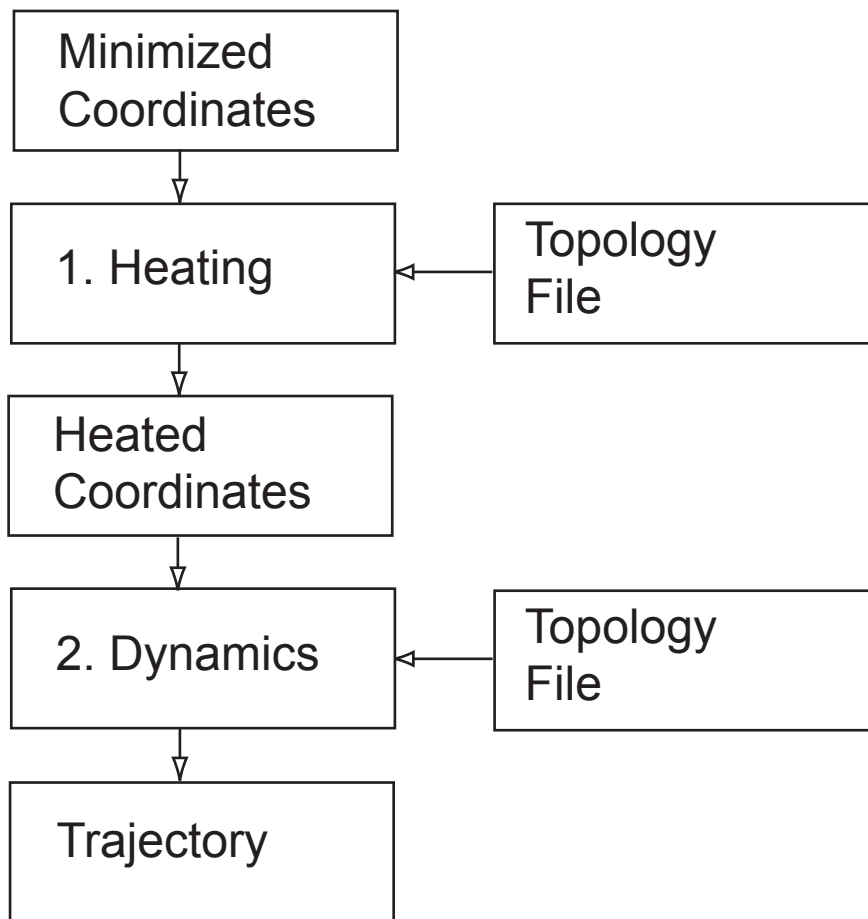
The initial (blue) and the final (red) geometry of the peptide, minimized with the interatomic constrain



MM dynamics of small proteins and nucleic acids

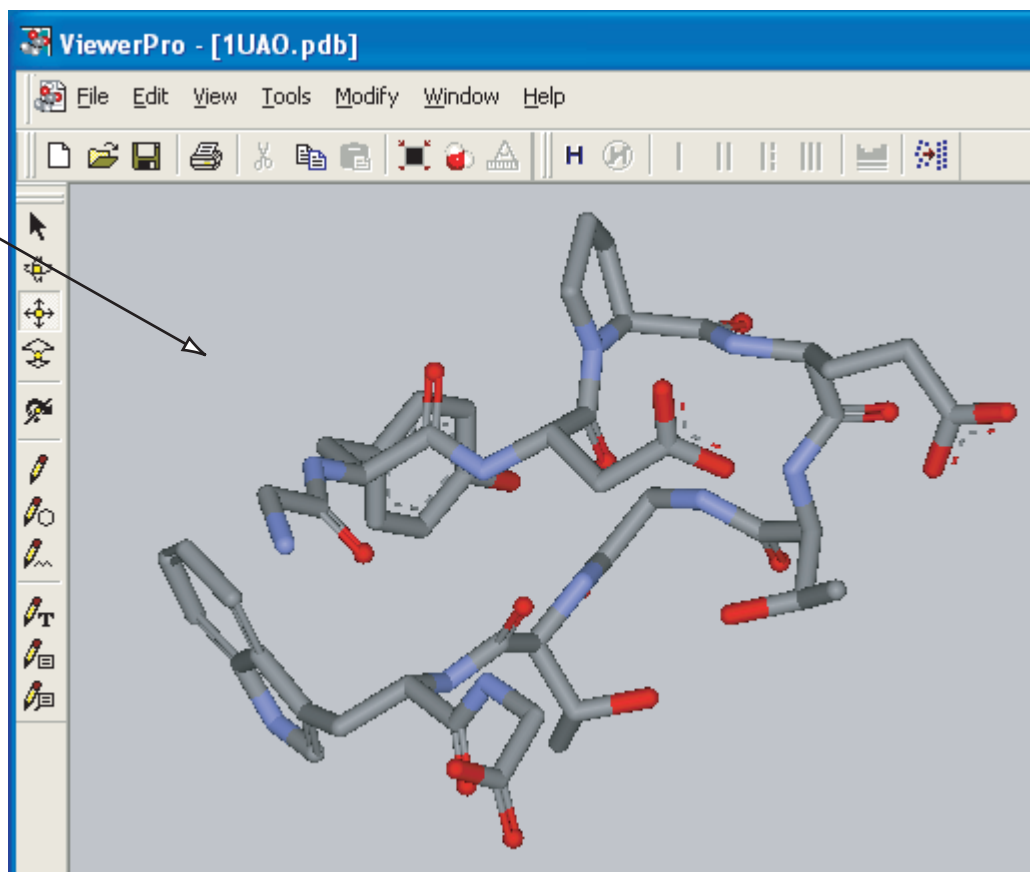
MM dynamics has
two steps: heating
and real dynamics

Each step requires
two files the topology
file and the initial
coordinates file



MM dynamics of Chignolin

Experimental
PDB structure
of Chignolin



MM dynamics of Chignolin

The PDB file of
Chignolin


Technical details
of experiment

Atomic
coordinates

```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
CRYST1      1.000      1.000      1.000  90.00  90.00  90.00 P 1
ORIGX1      1.000000   0.000000   0.000000      0.000000
ORIGX2      0.000000   1.000000   0.000000      0.000000
ORIGX3      0.000000   0.000000   1.000000      0.000000
SCALE1      1.000000   0.000000   0.000000      0.000000
SCALE2      0.000000   1.000000   0.000000      0.000000
SCALE3      0.000000   0.000000   1.000000      0.000000
MODEL       1
ATOM        1  N   GLY A   1      -6.778  -1.424   4.200  1.0
ATOM        2  CA  GLY A   1      -6.878  -0.708   2.896  1.0
ATOM        3  C   GLY A   1      -5.557  -0.840   2.138  1.0
ATOM        4  O   GLY A   1      -4.640  -1.504   2.579  1.0
Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 -
```

MM dynamics of Chignolin

The initial
coordinates in
a PDB format

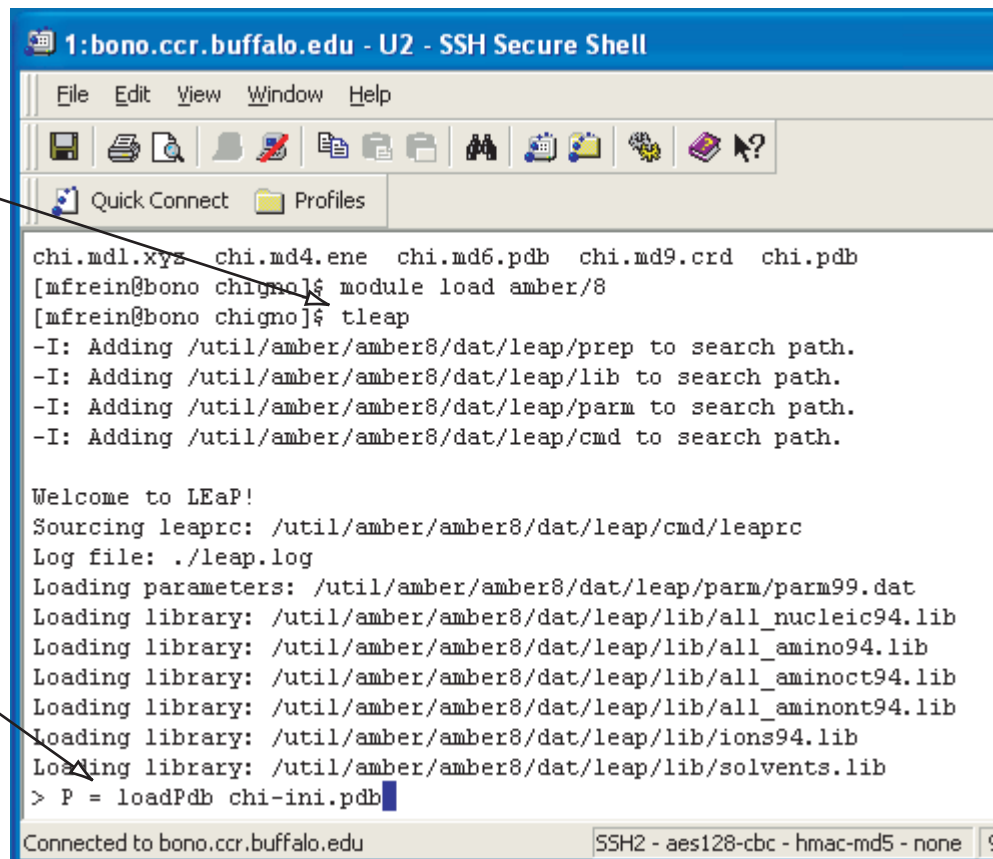


```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles
ATOM 1 N GLY A 1 -6.778 -1.424 4.200
ATOM 2 CA GLY A 1 -6.878 -0.708 2.896
ATOM 3 C GLY A 1 -5.557 -0.840 2.138
ATOM 4 O GLY A 1 -4.640 -1.504 2.579
ATOM 10 N TYR A 2 -5.452 -0.212 0.999
ATOM 11 CA TYR A 2 -4.189 -0.302 0.213
ATOM 12 C TYR A 2 -3.197 0.744 0.717
ATOM 13 O TYR A 2 -3.252 1.898 0.342
ATOM 14 CB TYR A 2 -4.490 -0.048 -1.264
ATOM 15 CG TYR A 2 -3.216 -0.141 -2.068
ATOM 16 CD1 TYR A 2 -2.780 -1.383 -2.544
ATOM 17 CD2 TYR A 2 -2.474 1.015 -2.342
"chi-ini.pdb" 78L, 6318C
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-m
```

MM dynamics of Chignolin

The Tleap program
generating
topology and
coordinates files

Loading the initial
coordinates



```
1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

chi.mdl.xyz chi.md4.ene chi.md6.pdb chi.md9.crd chi.pdb
[mfrein@bono chigno]$ module load amber/8
[mfrein@bono chigno]$ tleap
-I: Adding /util/amber/amber8/dat/leap/prep to search path.
-I: Adding /util/amber/amber8/dat/leap/lib to search path.
-I: Adding /util/amber/amber8/dat/leap/parm to search path.
-I: Adding /util/amber/amber8/dat/leap/cmd to search path.

Welcome to LEaP!
Sourcing leaprc: /util/amber/amber8/dat/leap/cmd/leaprc
Log file: ./leap.log
Loading parameters: /util/amber/amber8/dat/leap/parm/parm99.dat
Loading library: /util/amber/amber8/dat/leap/lib/all_nucleic94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_amino94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminoc94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminont94.lib
Loading library: /util/amber/amber8/dat/leap/lib/ions94.lib
Loading library: /util/amber/amber8/dat/leap/lib/solvents.lib
> P = loadPdb chi-ini.pdb
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 9
```

MM dynamics of Chignolin

Saving the initial
PDB files
(with hydrogens)

Saving the
topology and
coordinates files

```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

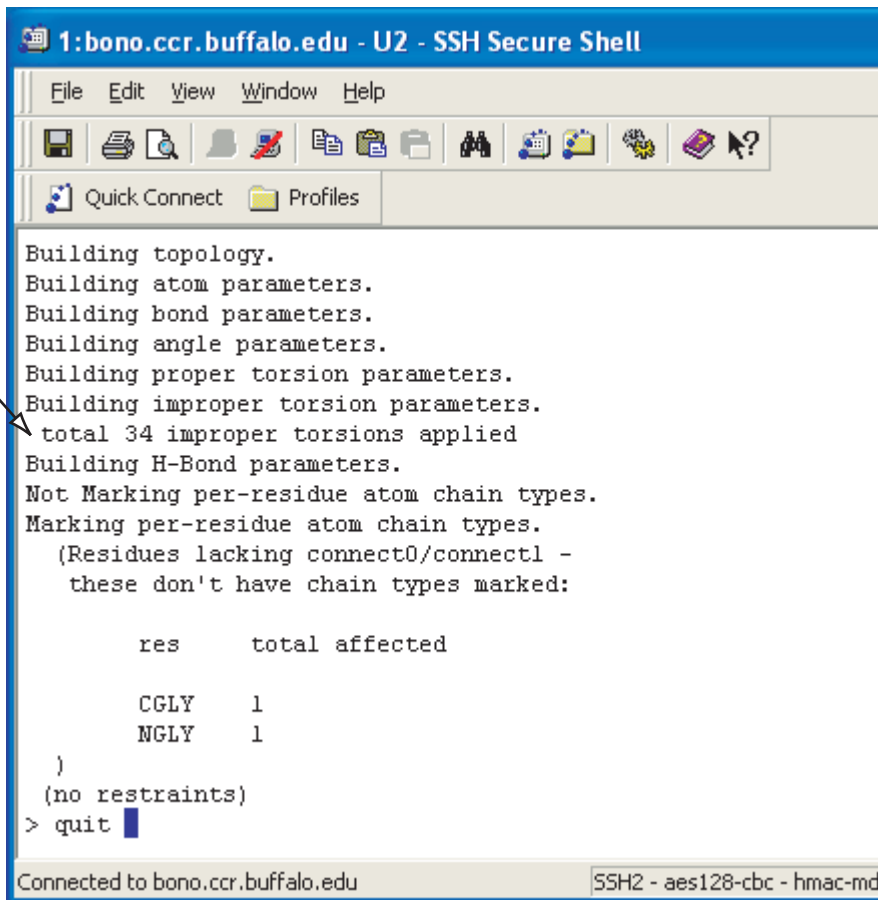
Sourcing leaprc: /util/amber/amber8/dat/leap/cmd/leaprc
Log file: ./leap.log
Loading parameters: /util/amber/amber8/dat/leap/parm/parm99.dat
Loading library: /util/amber/amber8/dat/leap/lib/all_nucleic94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_amino94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminoc94.lib
Loading library: /util/amber/amber8/dat/leap/lib/all_aminont94.lib
Loading library: /util/amber/amber8/dat/leap/lib/ions94.lib
Loading library: /util/amber/amber8/dat/leap/lib/solvents.lib
> P = loadPdb chi-ini.pdb
Loading PDB file: ./chi-ini.pdb
    total atoms in file: 77
    Leap added 61 missing atoms according to residue templates:
        61 H / lone pairs
> savePdb P chi.pdb
Writing pdb file: chi.pdb
    Shortening residue name for PDB format: NGLY -> GLY
    Shortening residue name for PDB format: CGLY -> GLY
> saveAmberParm P chi.top chi.xyz
```

Topology file

Coordinates file

MM dynamics of Chignolin

Building the
topology and
parameter data



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

Building topology.
Building atom parameters.
Building bond parameters.
Building angle parameters.
Building proper torsion parameters.
Building improper torsion parameters.
total 34 improper torsions applied
Building H-Bond parameters.
Not Marking per-residue atom chain types.
Marking per-residue atom chain types.
(Residues lacking connect0/connect1 -
these don't have chain types marked:

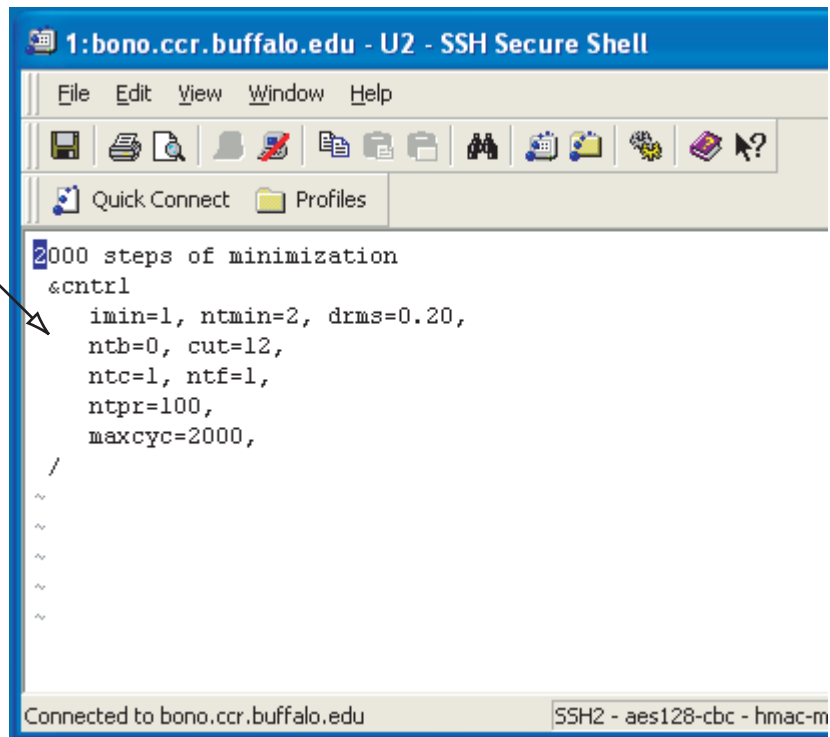
      res      total affected

      CGLY      1
      NGLY      1
)
(no restraints)
> quit
```

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md

MM dynamics of Chignolin

Technical details
of minimization



The screenshot shows a terminal window titled "1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window has a menu bar with "File", "Edit", "View", "Window", and "Help". Below the menu bar is a toolbar with various icons. The main text area displays the following content:

```
2000 steps of minimization
&ctrl
    imin=1, ntmin=2, drms=0.20,
    nth=0, cut=12,
    ntc=1, ntf=1,
    ntp=100,
    maxcyc=2000,
/
~
~
~
~
~
```

At the bottom of the window, a status bar indicates "Connected to bono.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-m".

MM dynamics of Chignolin

Technical details
of running
minimization

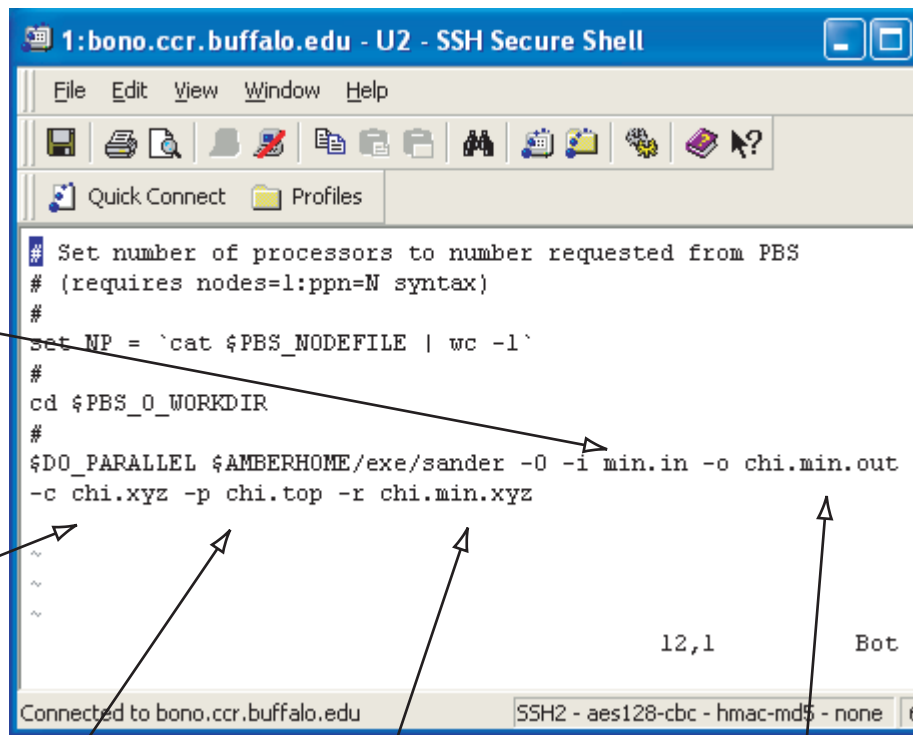
Input file of
minimization

Initial
coordinates

Topology file

Minimized
coordinates

Output file of
minimization



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i min.in -o chi.min.out
-c chi.xyz -p chi.top -r chi.min.xyz

~
~
~

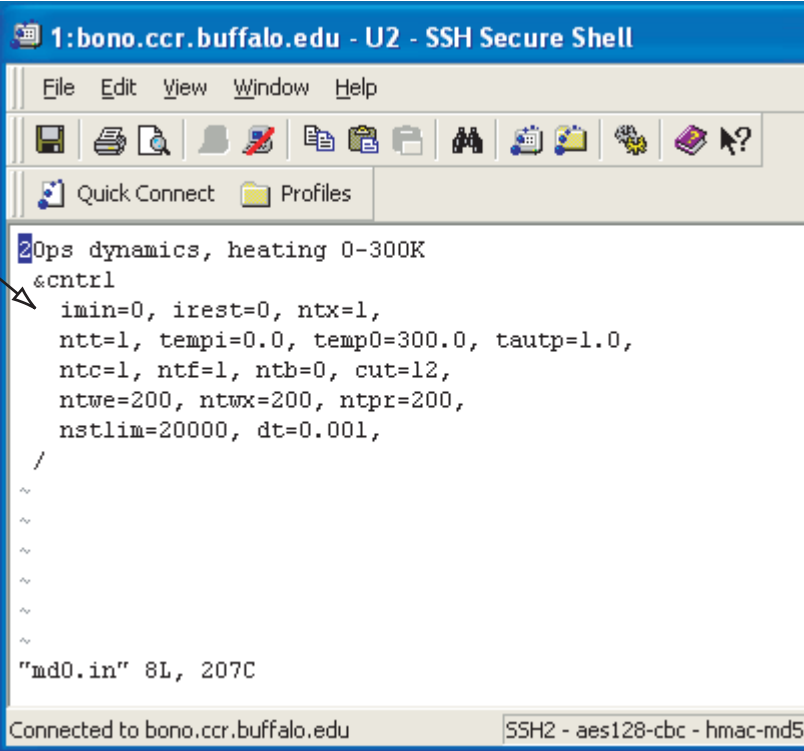
12,1 Bot
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none
```

The screenshot shows an SSH window with a script for running molecular dynamics minimization. Arrows from the text labels point to the following lines in the script:

- Input file of minimization** points to the line: `min.in` in the command `$DO_PARALLEL $AMBERHOME/exe/sander -O -i min.in -o chi.min.out`
- Initial coordinates** points to the line: `chi.xyz` in the command `-c chi.xyz -p chi.top -r chi.min.xyz`
- Topology file** points to the line: `chi.top` in the command `-c chi.xyz -p chi.top -r chi.min.xyz`
- Minimized coordinates** points to the line: `chi.min.out` in the command `-O -i min.in -o chi.min.out`
- Output file of minimization** points to the line: `chi.min.out` in the command `-O -i min.in -o chi.min.out`

MM dynamics of Chignolin

Technical details
of heating



The screenshot shows an SSH terminal window titled "1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window has a menu bar with "File", "Edit", "View", "Window", and "Help". Below the menu bar is a toolbar with various icons. The terminal content shows a prompt "2" followed by the command "Ops dynamics, heating 0-300K". The user then enters "&cntrl" followed by a series of parameters: "imin=0, irest=0, ntx=1, ntt=1, tempi=0.0, temp0=300.0, tautp=1.0, ntc=1, ntf=1, ntb=0, cut=12, ntwe=200, ntwx=200, ntpr=200, nstlim=20000, dt=0.001,". The prompt then changes to "/" and then to "~" several times. Finally, the prompt changes to "md0.in" and the output shows "8L, 207C". The status bar at the bottom indicates "Connected to bono.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-md5".

```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
2 Ops dynamics, heating 0-300K
&cntrl
  imin=0, irest=0, ntx=1,
  ntt=1, tempi=0.0, temp0=300.0, tautp=1.0,
  ntc=1, ntf=1, ntb=0, cut=12,
  ntwe=200, ntwx=200, ntpr=200,
  nstlim=20000, dt=0.001,
/
~
~
~
~
~
~
"md0.in" 8L, 207C
Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```

MM dynamics of Chignolin

Technical details
of running heating

Input file of
heating

Initial
coordinates

Topology file

Heated
coordinates

Output file of
heating

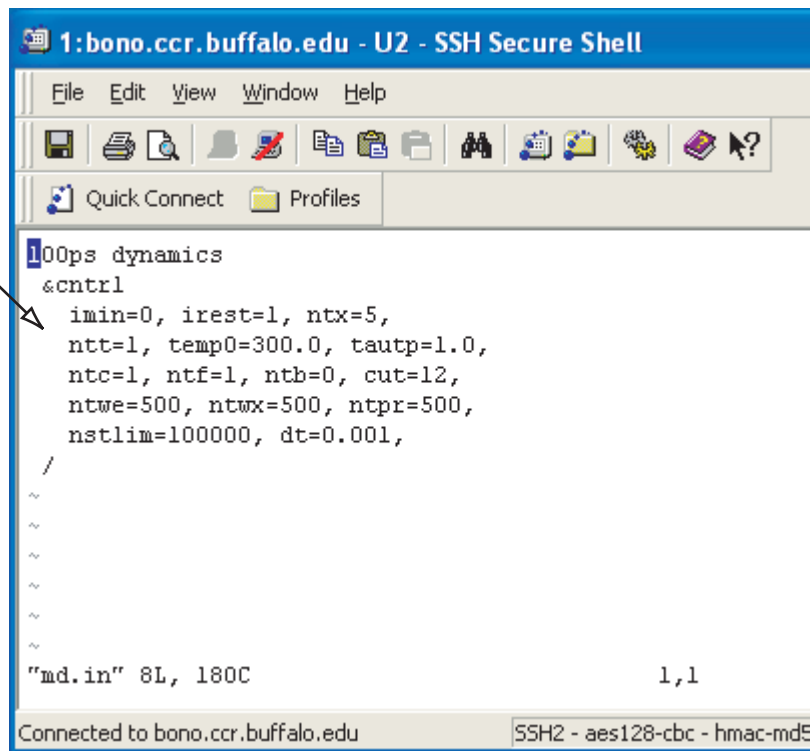
```
#
source $MODULESHOME/init/tcsh
module load amber/8
#
# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md0.in -o chi.md0.out
-c chi.min.xyz -p chi.top -r chi.md0.xyz
```

20,0-1 Bot

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac/md5 - none

MM dynamics of Chignolin

Technical details
of dynamics



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

100ps dynamics
&cntrl
    imin=0, irest=1, ntx=5,
    ntt=1, temp0=300.0, tautp=1.0,
    ntc=1, ntf=1, ntb=0, cut=12,
    ntwe=500, ntwx=500, ntpr=500,
    nstlim=100000, dt=0.001,
/
~
~
~
~
~
~
"md.in" 8L, 180C                                     1,1
Connected to bono.ccr.buffalo.edu                      SSH2 - aes128-cbc - hmac-md5
```

MM dynamics of Chignolin

Technical details
of running
dynamics

Input and output
files of dynamics

Initial
coordinates

Topology file

```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

module load amber/8
#
# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.mdl.out -c
chi.md0.xyz -p chi.top -r chi.mdl.xyz -x chi.mdl.crd -e chi.mdl.ene
@
9,19 47%
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 67x13
```

The screenshot shows an SSH terminal window titled "1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The terminal displays the execution of an Amber sander command. The command is: `$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.mdl.out -c chi.md0.xyz -p chi.top -r chi.mdl.xyz -x chi.mdl.crd -e chi.mdl.ene`. The output shows the command is running, with a progress bar indicating 9,19 and 47% completion. The terminal also shows the connection details: "Connected to bono.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-md5 - none 67x13".

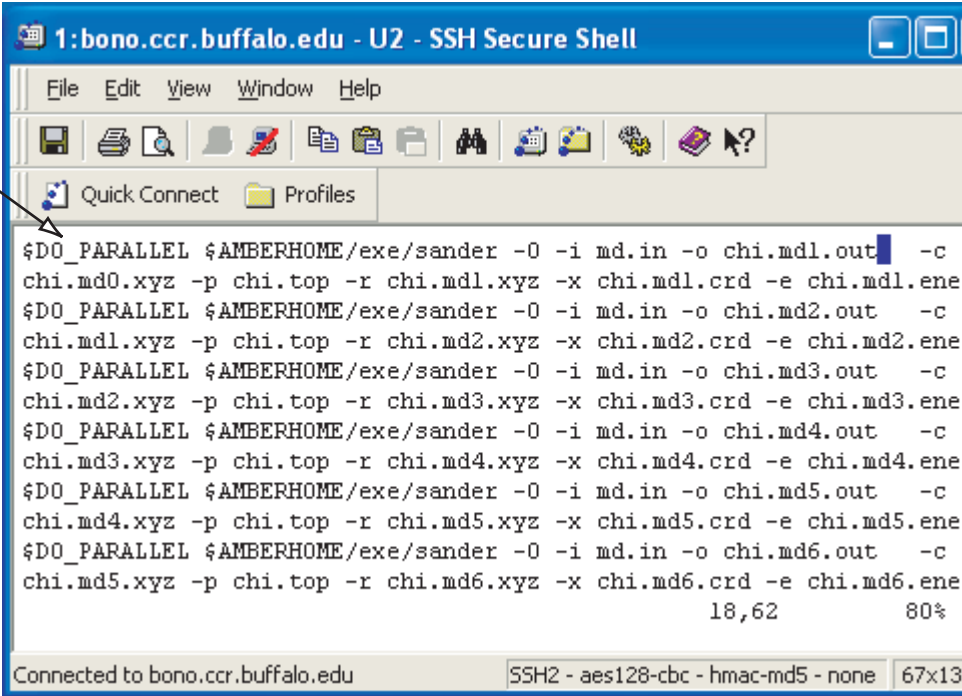
Final
coordinates

Complete
trajectory

Energy
components

MM dynamics of Chignolin

Technical details
of running several
steps of the same
dynamics



The screenshot shows an SSH terminal window titled "1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window has a menu bar with "File", "Edit", "View", "Window", and "Help". Below the menu bar is a toolbar with various icons. The main area of the terminal displays a series of commands being executed in a loop, indicated by the "\$DO_PARALLEL" prefix. The commands are for running molecular dynamics simulations using the "sander" program. The output shows the progress of the simulations, with the last line indicating "18,62" and "80%".

```
1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md1.out -c
chi.md0.xyz -p chi.top -r chi.md1.xyz -x chi.md1.crd -e chi.md1.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md2.out -c
chi.md1.xyz -p chi.top -r chi.md2.xyz -x chi.md2.crd -e chi.md2.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md3.out -c
chi.md2.xyz -p chi.top -r chi.md3.xyz -x chi.md3.crd -e chi.md3.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md4.out -c
chi.md3.xyz -p chi.top -r chi.md4.xyz -x chi.md4.crd -e chi.md4.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md5.out -c
chi.md4.xyz -p chi.top -r chi.md5.xyz -x chi.md5.crd -e chi.md5.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md6.out -c
chi.md5.xyz -p chi.top -r chi.md6.xyz -x chi.md6.crd -e chi.md6.ene
18,62 80%
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 67x13
```

MM dynamics of Chignolin

Energy
components
after 820ps

1: bono.ccr.buffalo.edu - U2 - SSH Secure Shell

File Edit View Window Help

Quick Connect Profiles

	Nsteps	time(ps)	Etot	EKinetic	
L1	Temp	T_solute	T_solv	Pres_scal_solu	
L2	Pres_scal_solv	BoxX	BoxY	BoxZ	
L3	volume	pres_X	pres_Y	pres_Z	
L4	Pressure	EKCoM_x	EKCoM_y	EKCoM_z	
L5	EKComTot	VIRIAL_x	VIRIAL_y	VIRIAL_z	
L6	VIRIAL_tot	E_pot	E_vdw	E_el	
L7	E_hbon	E_bon	E_angle	E_dih	
L8	E_l4vdw	E_l4el	E_const	E_pol	
L9	AV_permMoment	AV_indMoment	AV_totMoment	Density	dV/dlambda
L0	500	0.8205000000E+03	-.2594031443E+02	0.1192492155E+03	
L1	0.2941613449E+03	0.2941613449E+03	-.2833386442E+08	0.1000000000E+01	
L2	0.1000000000E+01	0.7335636390E+02	0.7254458130E+02	0.7262382620E+02	
L3	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	
L4	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	
L5	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	
L6	0.0000000000E+00	-.1451895299E+03	-.3552134856E+02	-.8926011656E+03	
L7	0.0000000000E+00	0.4982857510E+02	0.7787623366E+02	0.9669051708E+02	
L8	0.3452260295E+02	0.5240150555E+03	0.0000000000E+00	0.0000000000E+00	
L9	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	0.0000000000E+00	0.000000 1,1

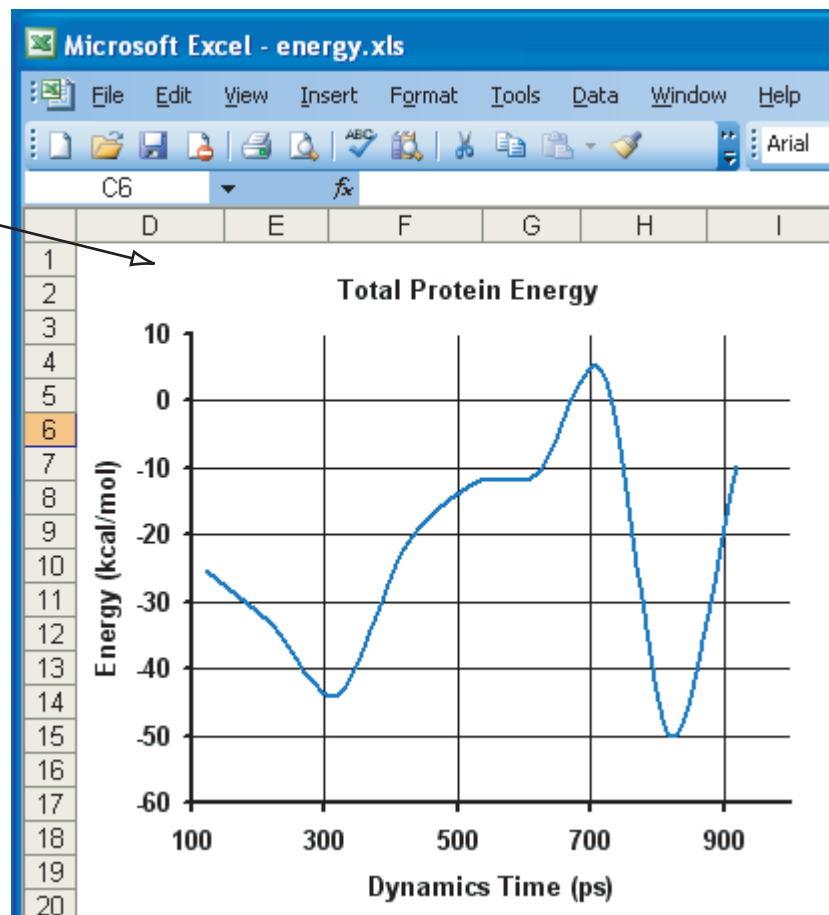
Connected to bono.ccr.buffalo.edu

SSH2 - aes128-cbc - hmac-md5 - none

91x21

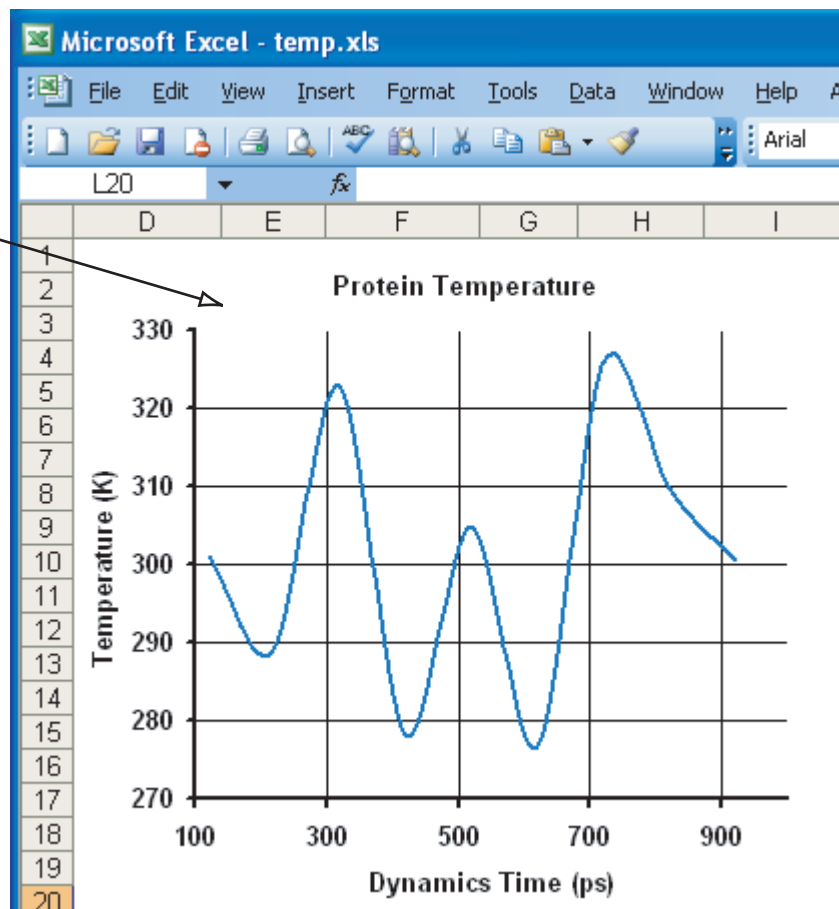
MM dynamics of Chignolin

Total energy of the protein as a function of dynamics time



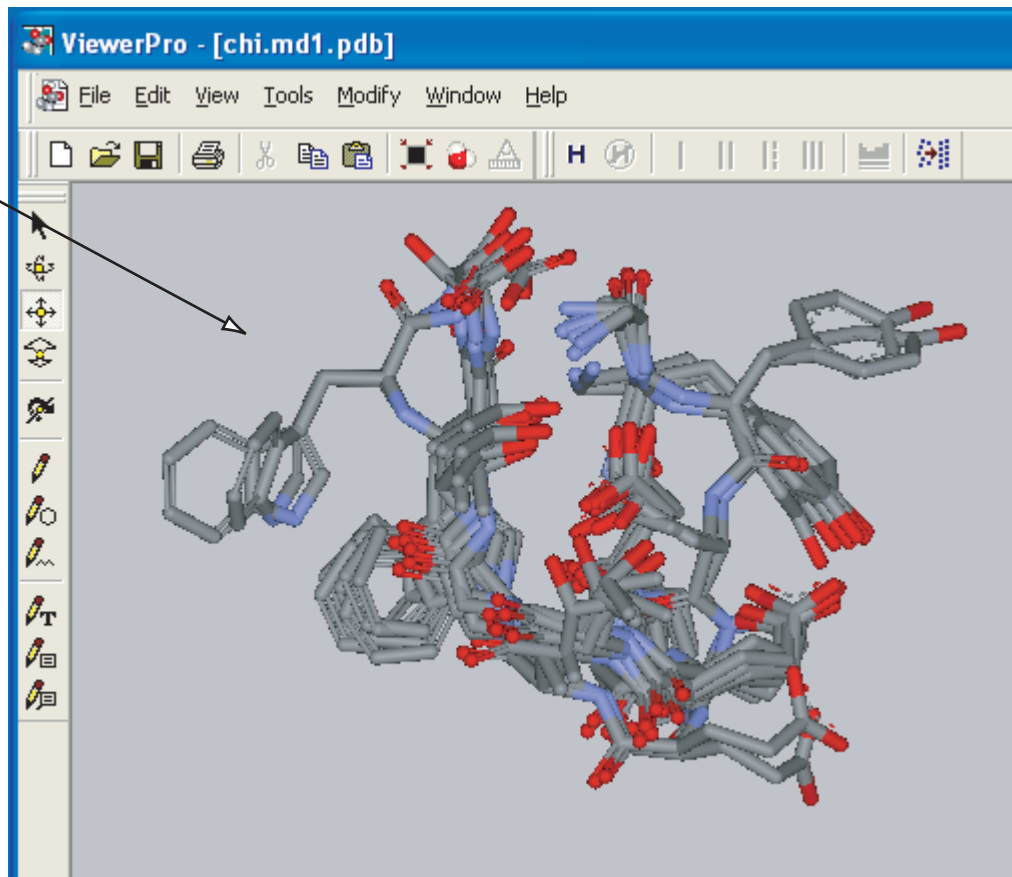
MM dynamics of Chignolin

Temperature of the protein as a function of dynamics time



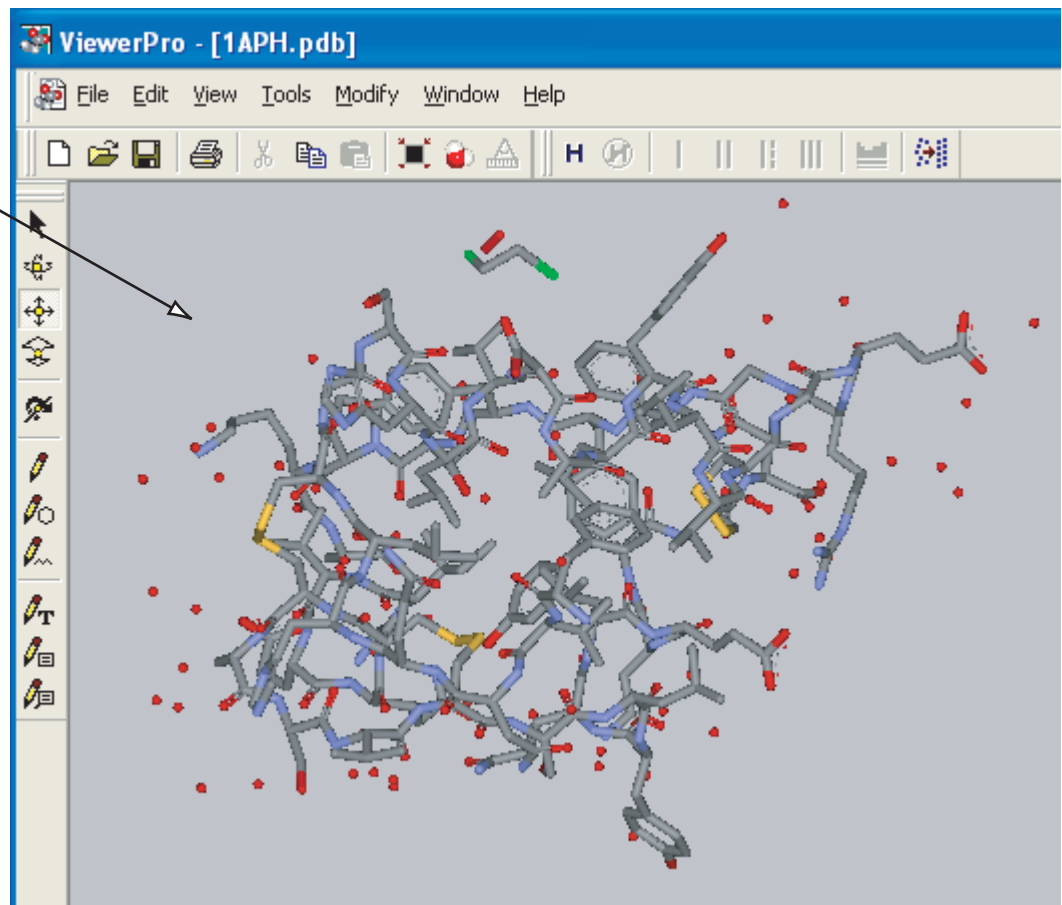
MM dynamics of Chignolin

Superposition of
10 protein
structures obtained
from 1ns dynamics



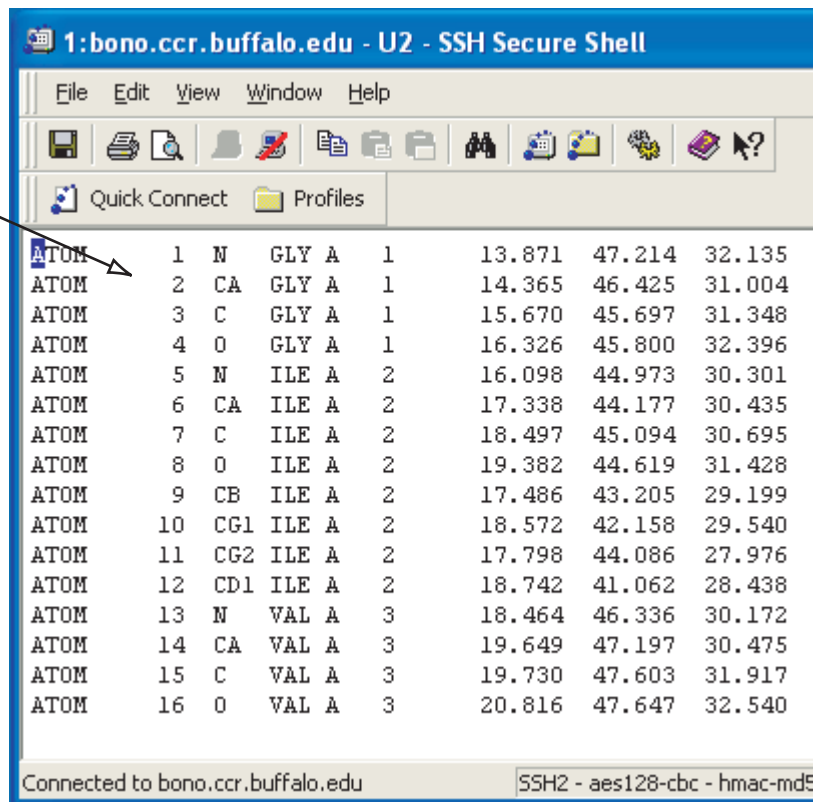
MM dynamics of Insulin

Experimental
PDB structure
of Insulin



MM dynamics of Insulin

Modified PDB file of
insulin
(no crystallographic
water molecules)



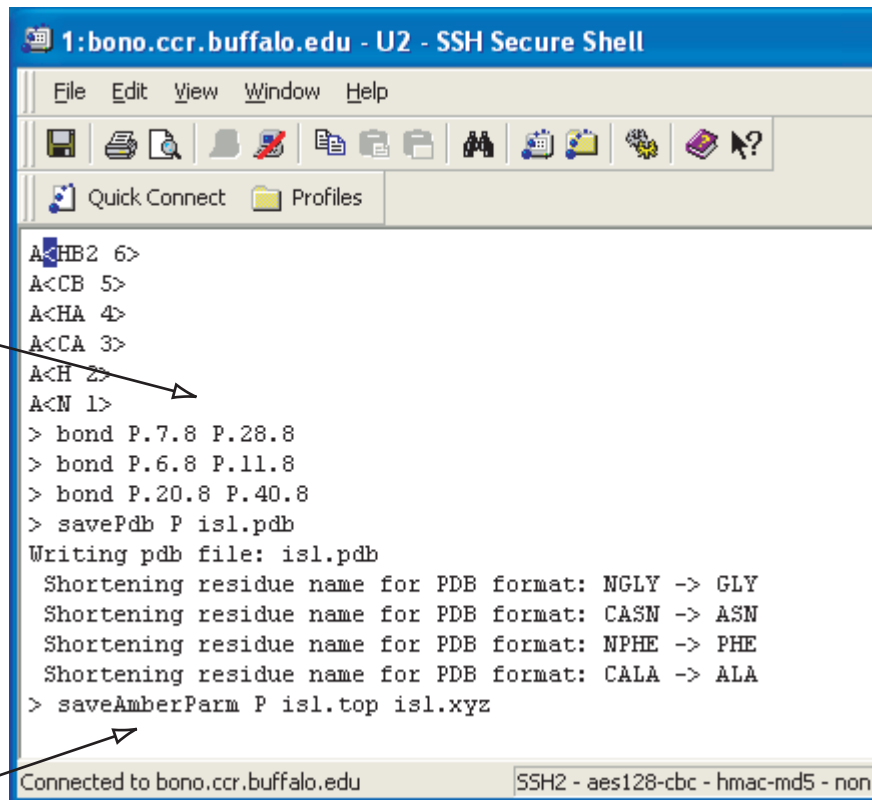
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell							
File Edit View Window Help							
Quick Connect Profiles							
ATOM	1	N	GLY	A	1	13.871	47.214 32.135
ATOM	2	CA	GLY	A	1	14.365	46.425 31.004
ATOM	3	C	GLY	A	1	15.670	45.697 31.348
ATOM	4	O	GLY	A	1	16.326	45.800 32.396
ATOM	5	N	ILE	A	2	16.098	44.973 30.301
ATOM	6	CA	ILE	A	2	17.338	44.177 30.435
ATOM	7	C	ILE	A	2	18.497	45.094 30.695
ATOM	8	O	ILE	A	2	19.382	44.619 31.428
ATOM	9	CB	ILE	A	2	17.486	43.205 29.199
ATOM	10	CG1	ILE	A	2	18.572	42.158 29.540
ATOM	11	CG2	ILE	A	2	17.798	44.086 27.976
ATOM	12	CD1	ILE	A	2	18.742	41.062 28.438
ATOM	13	N	VAL	A	3	18.464	46.336 30.172
ATOM	14	CA	VAL	A	3	19.649	47.197 30.475
ATOM	15	C	VAL	A	3	19.730	47.603 31.917
ATOM	16	O	VAL	A	3	20.816	47.647 32.540
Connected to bono.ccr.buffalo.edu					SSH2 - aes128-cbc - hmac-md5		

MM dynamics of Insulin

Bonding cysteine
amino acids in the
tlep program

- Unit name
- Residue number
- Atom number

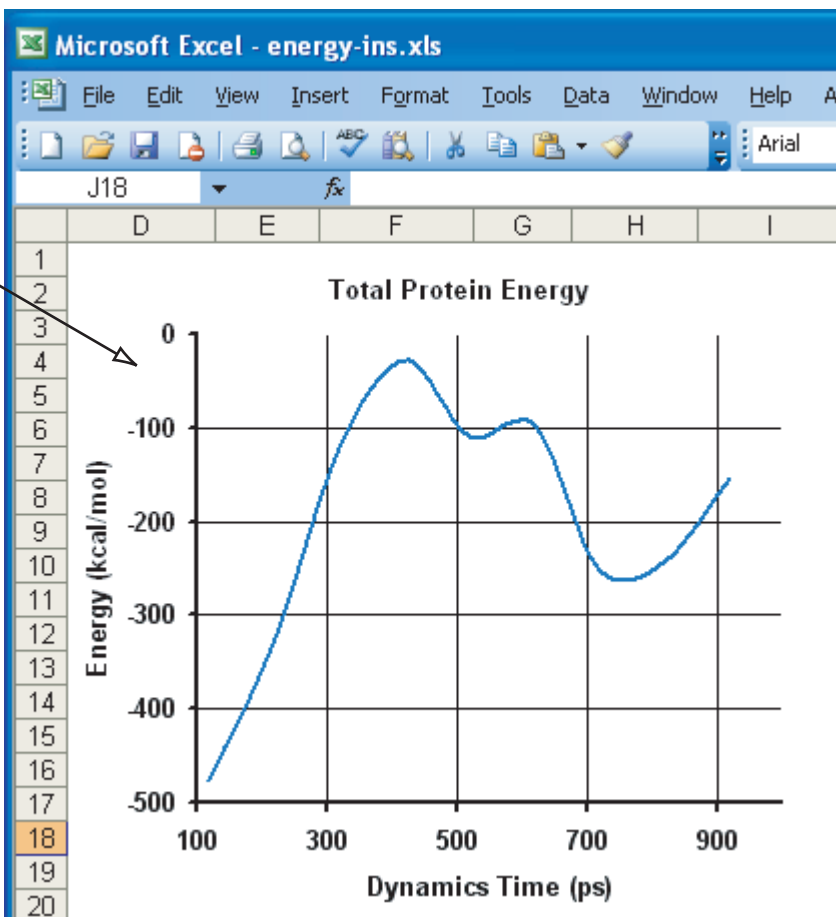
Saving the topology
and coordinates files
with sulfur bridges



```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
A<HB2 6>
A<CB 5>
A<HA 4>
A<CA 3>
A<H 2>
A<N 1>
> bond P.7.8 P.28.8
> bond P.6.8 P.11.8
> bond P.20.8 P.40.8
> savePdb P isl.pdb
Writing pdb file: isl.pdb
Shortening residue name for PDB format: NGLY -> GLY
Shortening residue name for PDB format: CASN -> ASN
Shortening residue name for PDB format: NPHE -> PHE
Shortening residue name for PDB format: CALA -> ALA
> saveAmberParm P isl.top isl.xyz
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - non
```

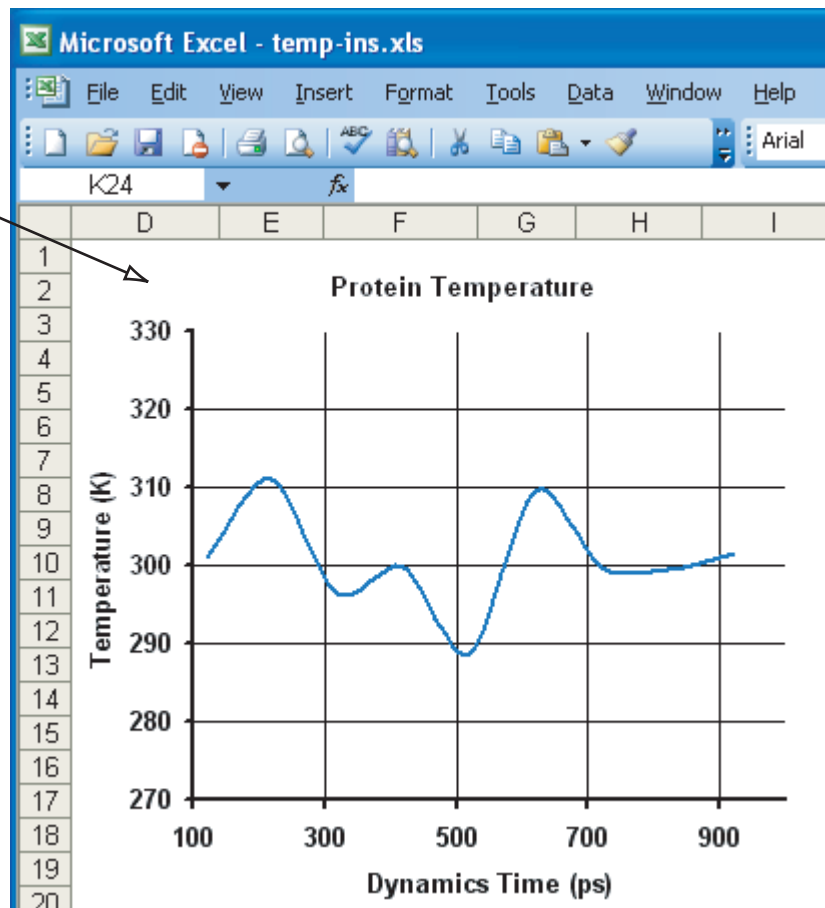
MM dynamics of Insulin

The total energy of the protein as a function of dynamics time



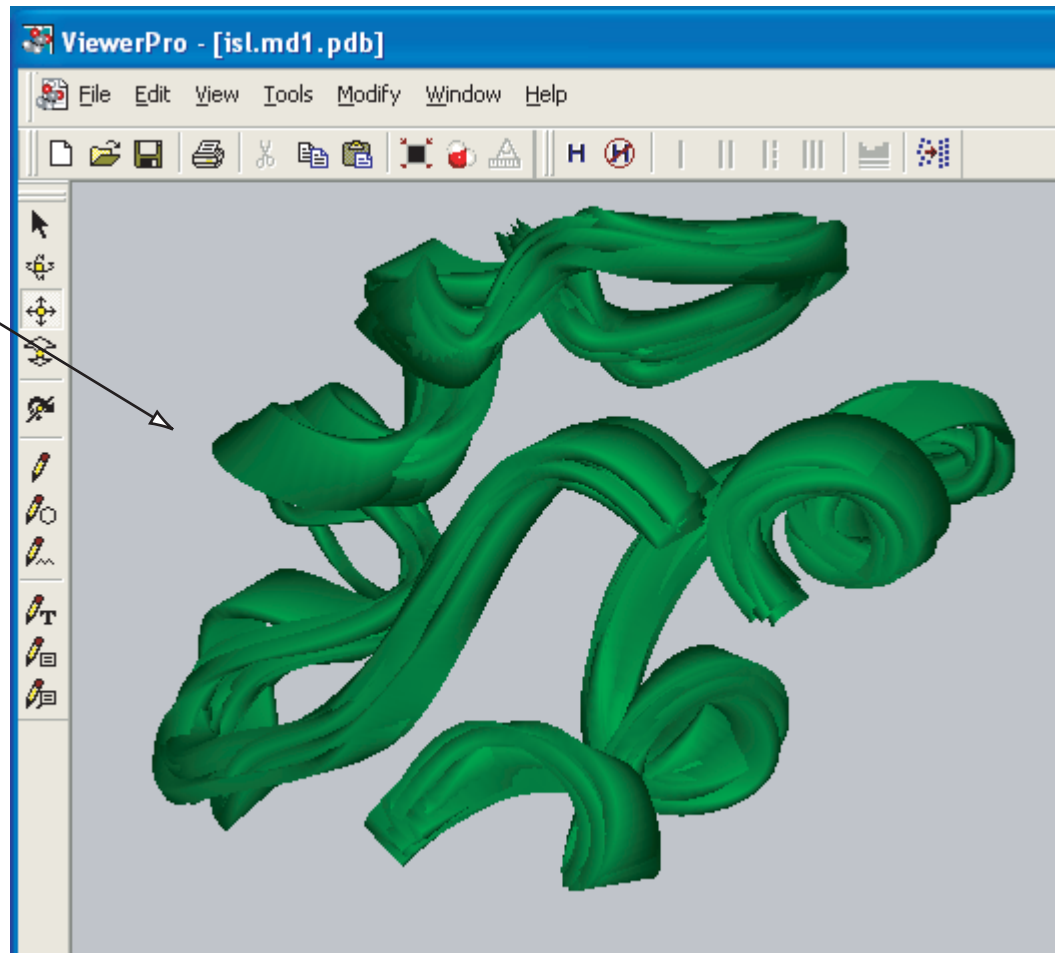
MM dynamics of Insulin

Temperature of the protein as a function of dynamics time



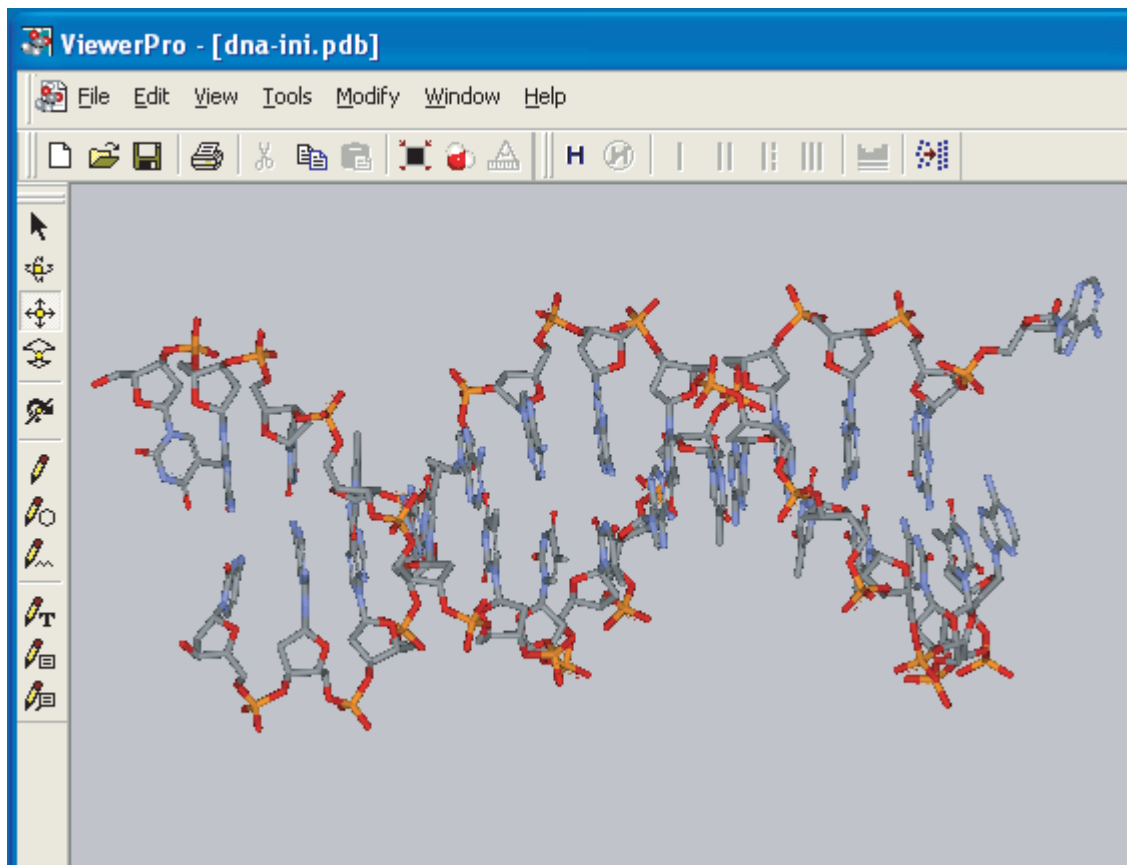
MM dynamics of Insulin

Superposition
of 10 protein
structures
obtained from
1ns dynamics



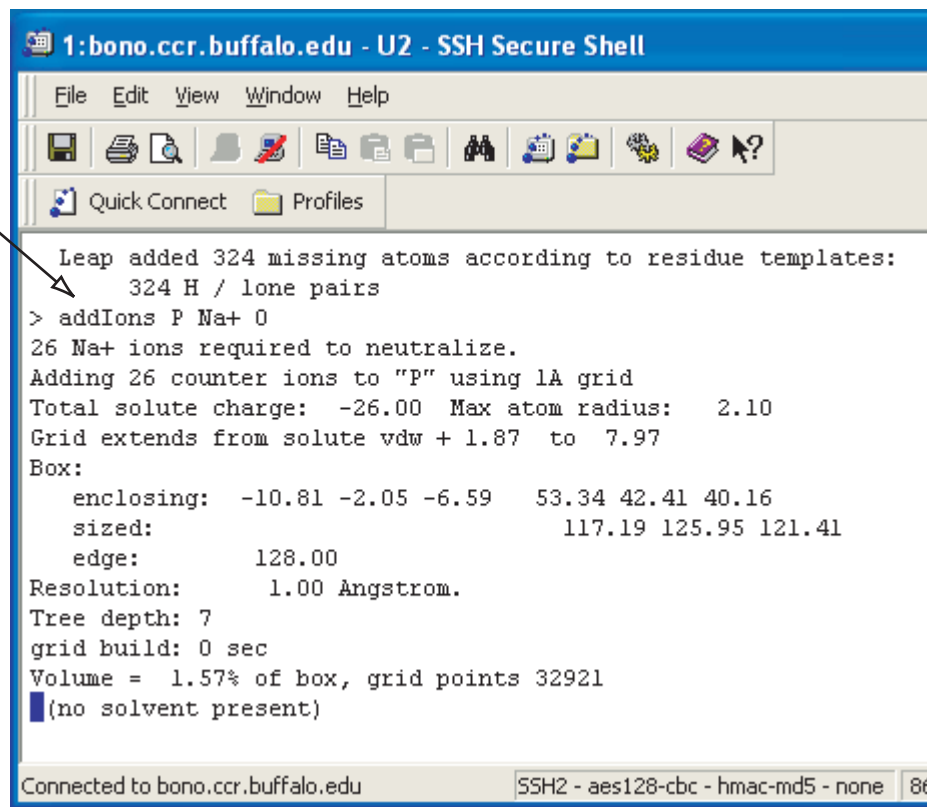
MM dynamics of DNA

Experimental
PDB
structure of a
small DNA



MM dynamics of DNA

Adding sodium cations to neutralize the nucleic acid, in the tleap program



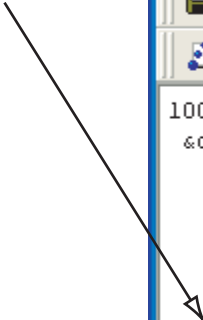
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

Leap added 324 missing atoms according to residue templates:
  324 H / lone pairs
> addIons P Na+ 0
26 Na+ ions required to neutralize.
Adding 26 counter ions to "P" using 1A grid
Total solute charge: -26.00 Max atom radius: 2.10
Grid extends from solute vdw + 1.87 to 7.97
Box:
  enclosing: -10.81 -2.05 -6.59 53.34 42.41 40.16
  sized: 117.19 125.95 121.41
  edge: 128.00
Resolution: 1.00 Angstrom.
Tree depth: 7
grid build: 0 sec
Volume = 1.57% of box, grid points 32921
[no solvent present]

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 86
```

MM dynamics of DNA

Minimization with
constrained
positions of
phosphorus and
sodium atoms



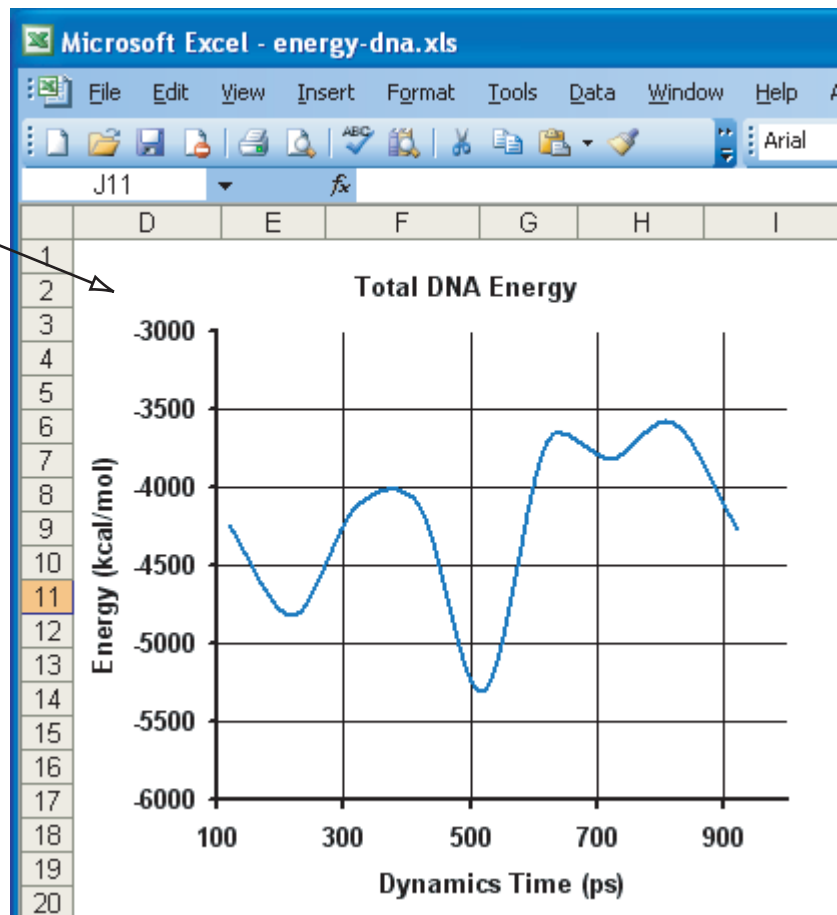
```
1:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

1000 steps of minimization
&cntrl
    imin=1, ntmin=2, drms=0.20,
    ntb=0, cut=12,
    ntc=1, ntf=1,
    ntpr=100,
    maxcyc=1000,
    ntr=1,
    restraint_wt=500.0,
    restraintmask='(@P=) | (:Na+)',
/

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - r
```

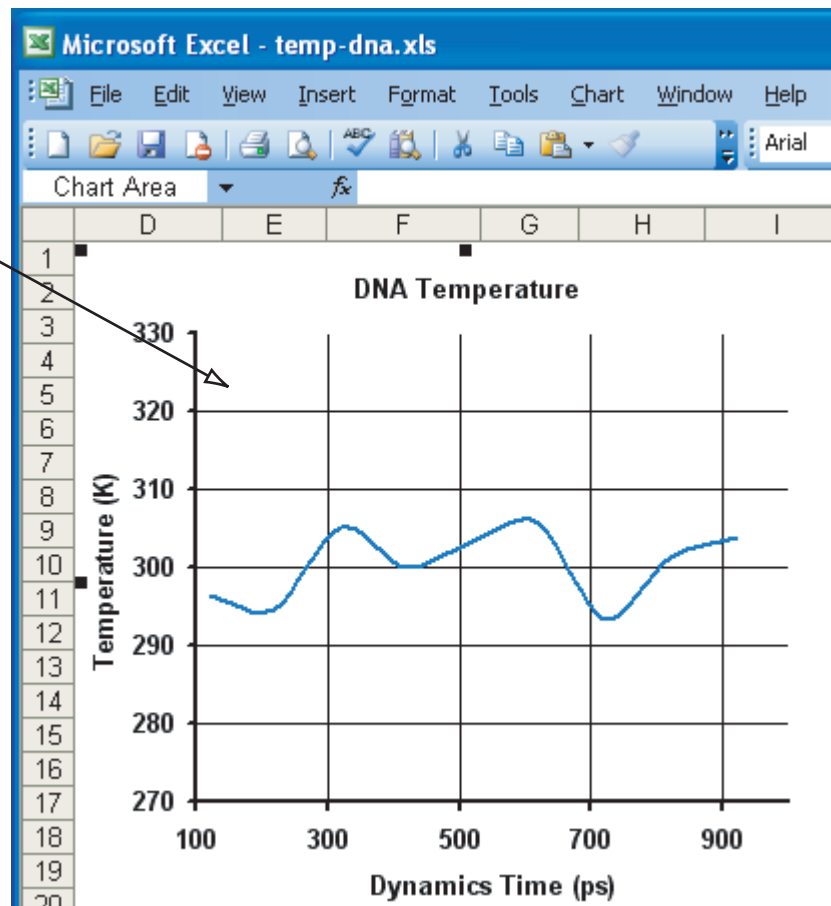
MM dynamics of DNA

Total DNA energy
as a function of
dynamics time



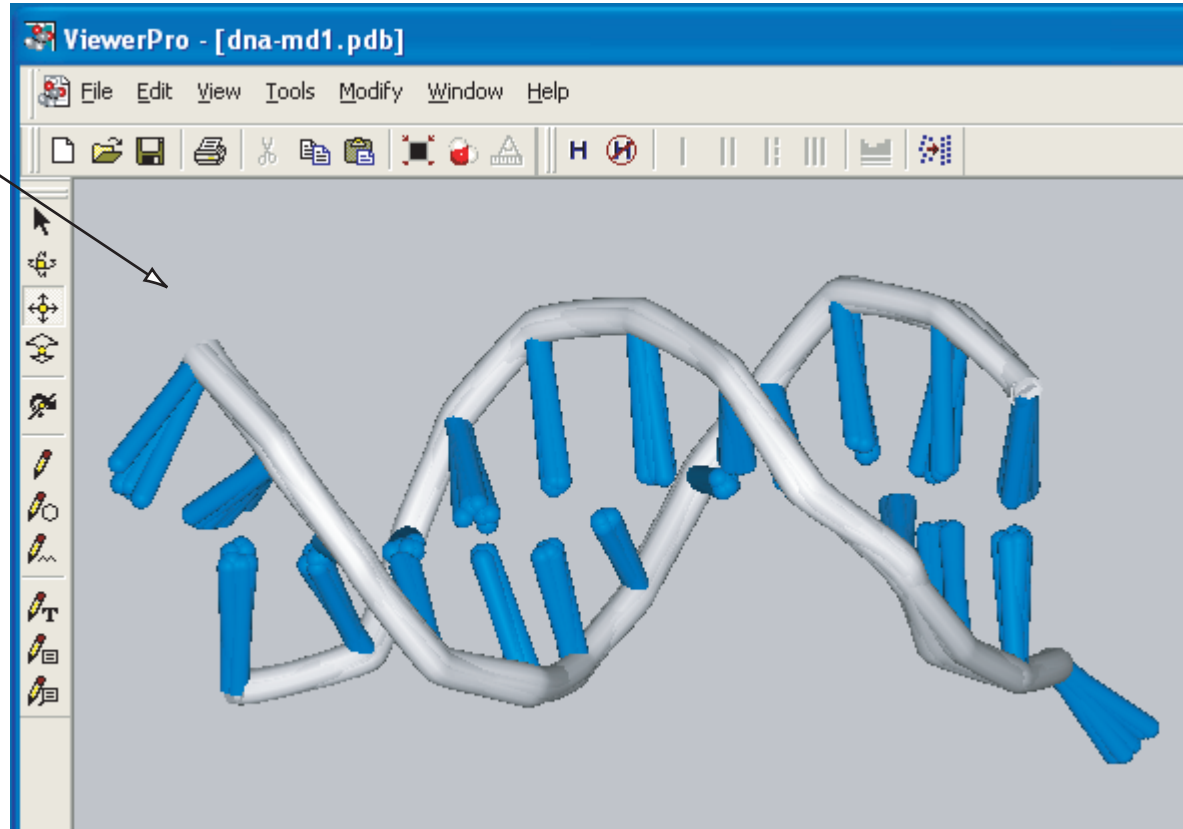
MM dynamics of DNA

DNA temperature
as a function of
dynamics time



MM dynamics of DNA

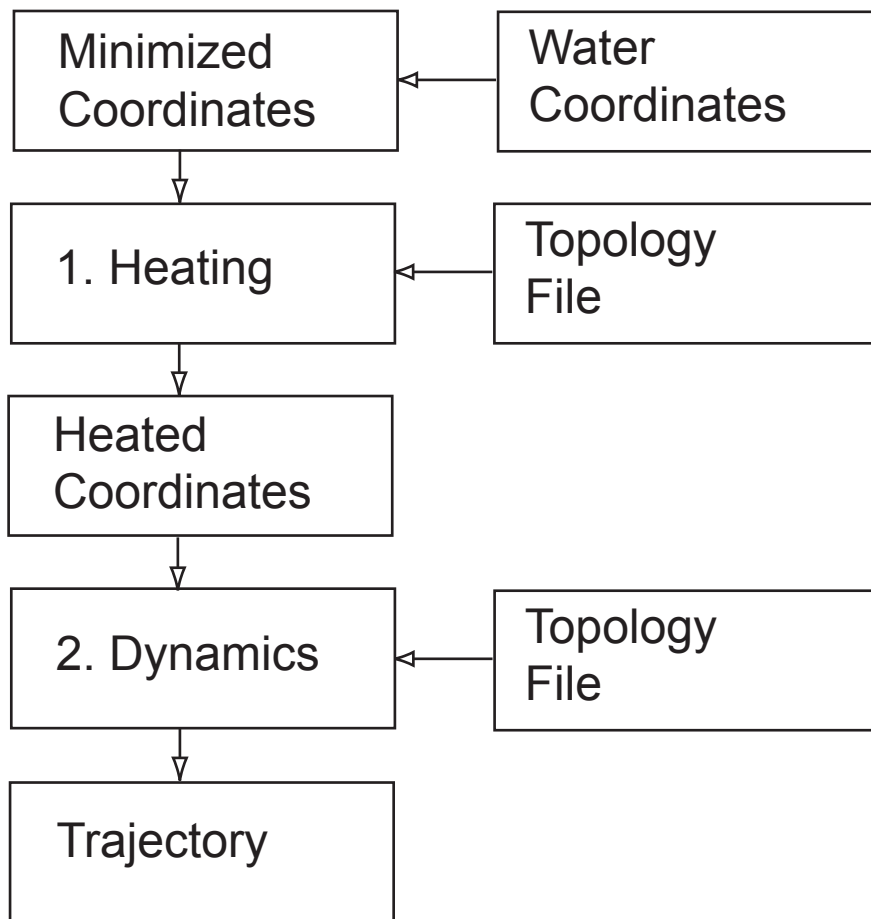
Superposition
of 10 DNA
structures
after 1ns
dynamics
temperature



MM dynamics in water solution

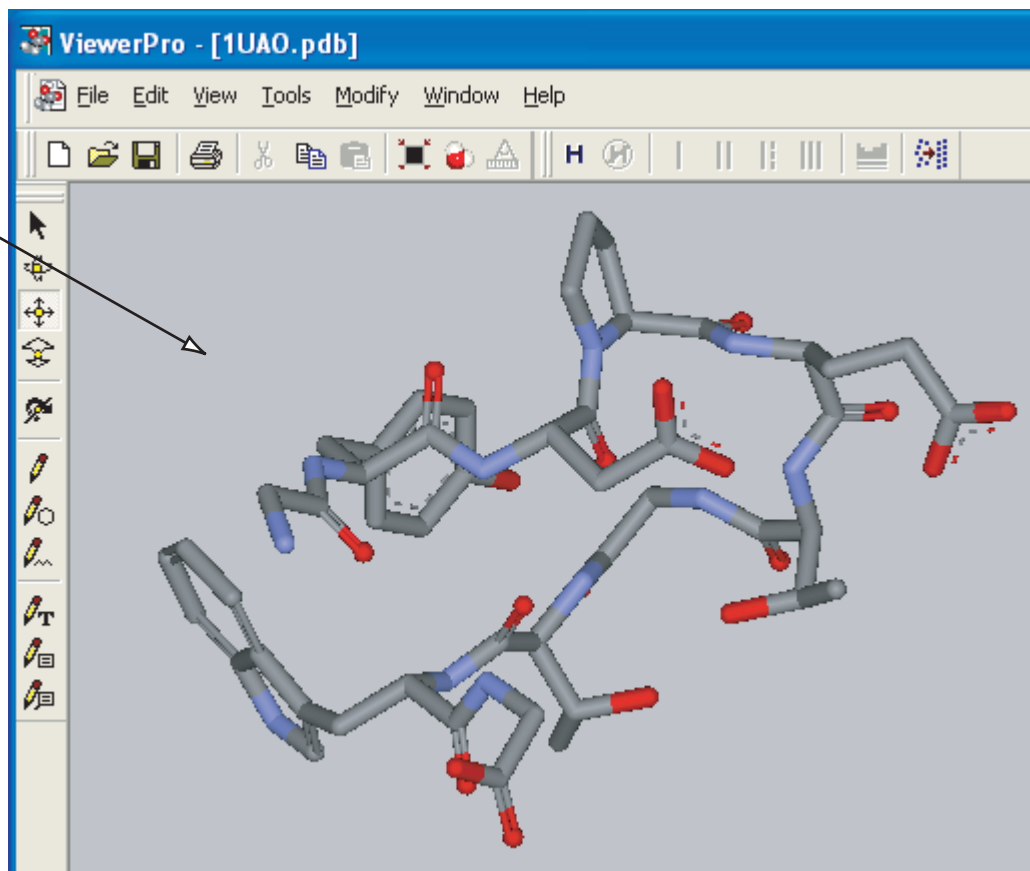
MM dynamics in water solution can be performed using implicit or explicit water molecules

MM dynamics with explicit water molecules used a TIP3P water model



MM dynamics of Chignolin in a sphere of water

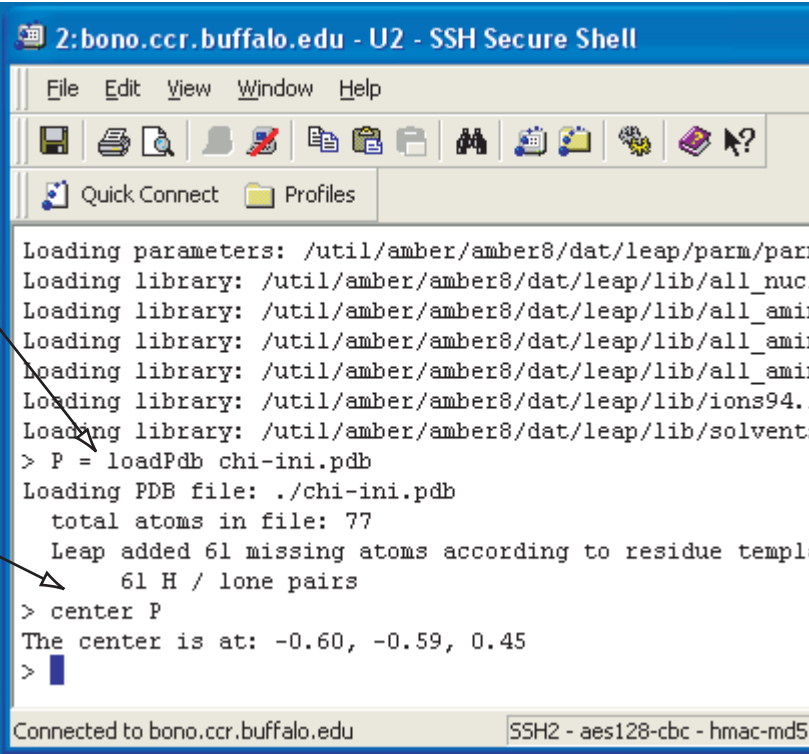
Experimental
PDB structure
of Chignolin



MM dynamics of Chignolin in a sphere of water

Loading the initial
PDB file of the protein

Finding the center of
the protein



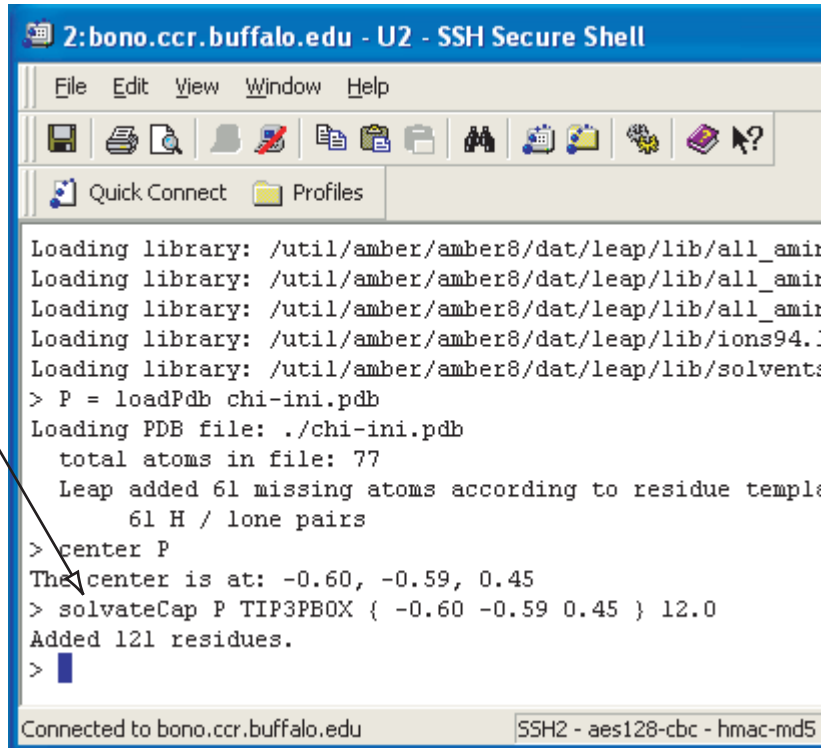
```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

Loading parameters: /util/amber/amber8/dat/leap/parm/par
Loading library: /util/amber/amber8/dat/leap/lib/all_nuc
Loading library: /util/amber/amber8/dat/leap/lib/all_ami
Loading library: /util/amber/amber8/dat/leap/lib/all_ami
Loading library: /util/amber/amber8/dat/leap/lib/all_ami
Loading library: /util/amber/amber8/dat/leap/lib/ions94.
Loading library: /util/amber/amber8/dat/leap/lib/solvents
> P = loadPdb chi-ini.pdb
Loading PDB file: ./chi-ini.pdb
      total atoms in file: 77
      Leap added 61 missing atoms according to residue templ
        61 H / lone pairs
> center P
The center is at: -0.60, -0.59, 0.45
> █

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```

MM dynamics of Chignolin in a sphere of water

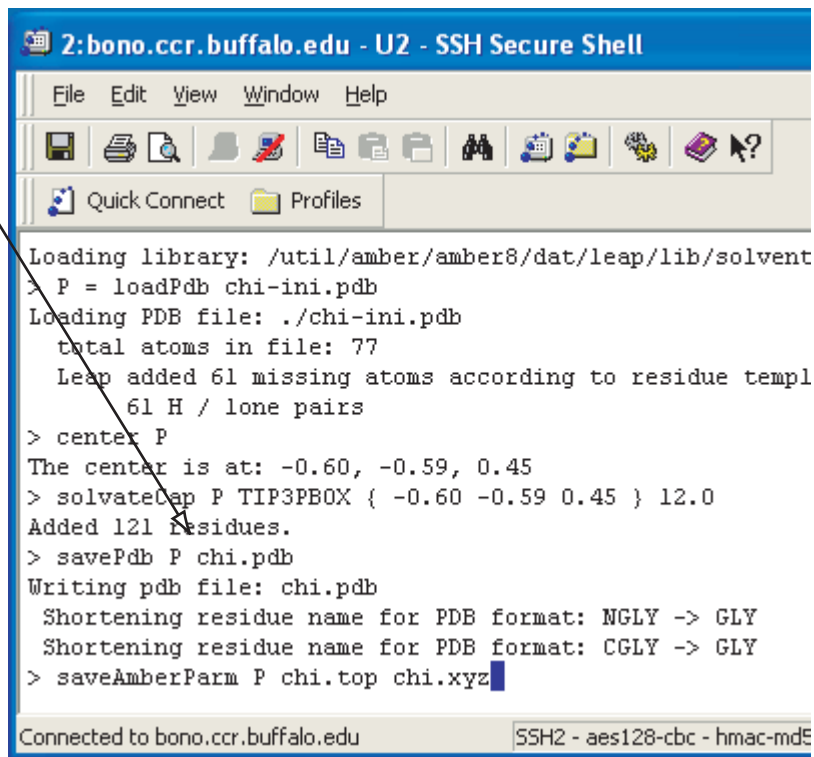
Solvating the protein
by a sphere of explicit
water molecules, of a
radius 12Å



```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
Loading library: /util/amber/amber8/dat/leap/lib/all_ami
Loading library: /util/amber/amber8/dat/leap/lib/all_ami
Loading library: /util/amber/amber8/dat/leap/lib/all_ami
Loading library: /util/amber/amber8/dat/leap/lib/ions94.
Loading library: /util/amber/amber8/dat/leap/lib/solvent:
> P = loadPdb chi-ini.pdb
Loading PDB file: ./chi-ini.pdb
total atoms in file: 77
Leap added 61 missing atoms according to residue templ
61 H / lone pairs
> center P
The center is at: -0.60, -0.59, 0.45
> solvateCap P TIP3PBOX { -0.60 -0.59 0.45 } 12.0
Added 121 residues.
>
Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5
```

MM dynamics of Chignolin in a sphere of water

Saving the PDB, the topology and the initial coordinates files



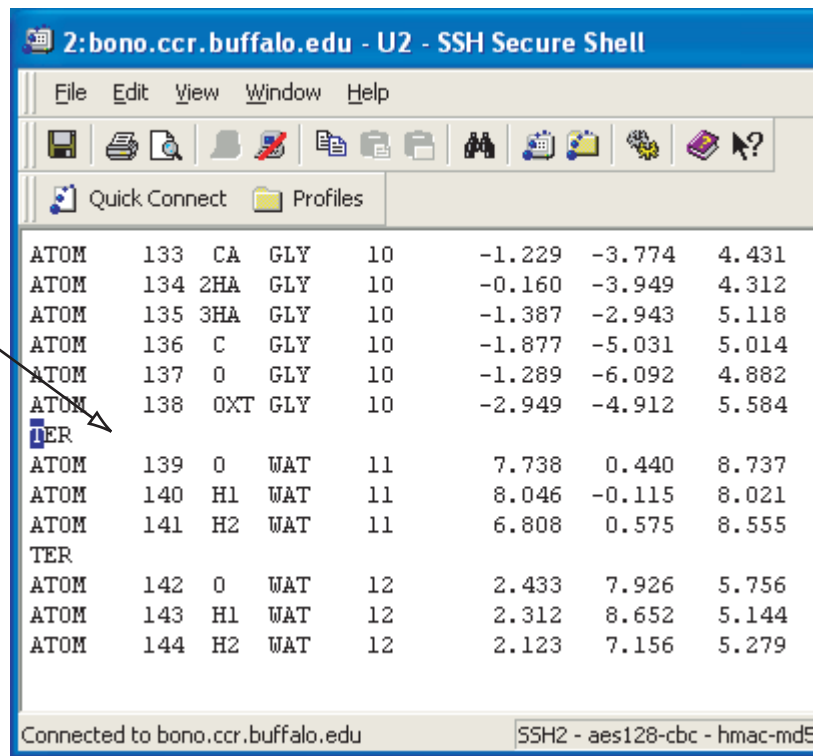
```
2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell
File Edit View Window Help
[Icons]
Quick Connect Profiles

Loading library: /util/amber/amber8/dat/leap/lib/solvent
> P = loadPdb chi-ini.pdb
Loading PDB file: ./chi-ini.pdb
  total atoms in file: 77
  Leap added 61 missing atoms according to residue template
  61 H / lone pairs
> center P
The center is at: -0.60, -0.59, 0.45
> solvateCap P TIP3PBOX { -0.60 -0.59 0.45 } 12.0
Added 121 residues.
> savePdb P chi.pdb
Writing pdb file: chi.pdb
  Shortening residue name for PDB format: NGLY -> GLY
  Shortening residue name for PDB format: CGLY -> GLY
> saveAmberParm P chi.top chi.xyz

Connected to bono.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```

MM dynamics of Chignolin in a sphere of water

The coordinates of
TIP3P water
molecules in the
PDB file



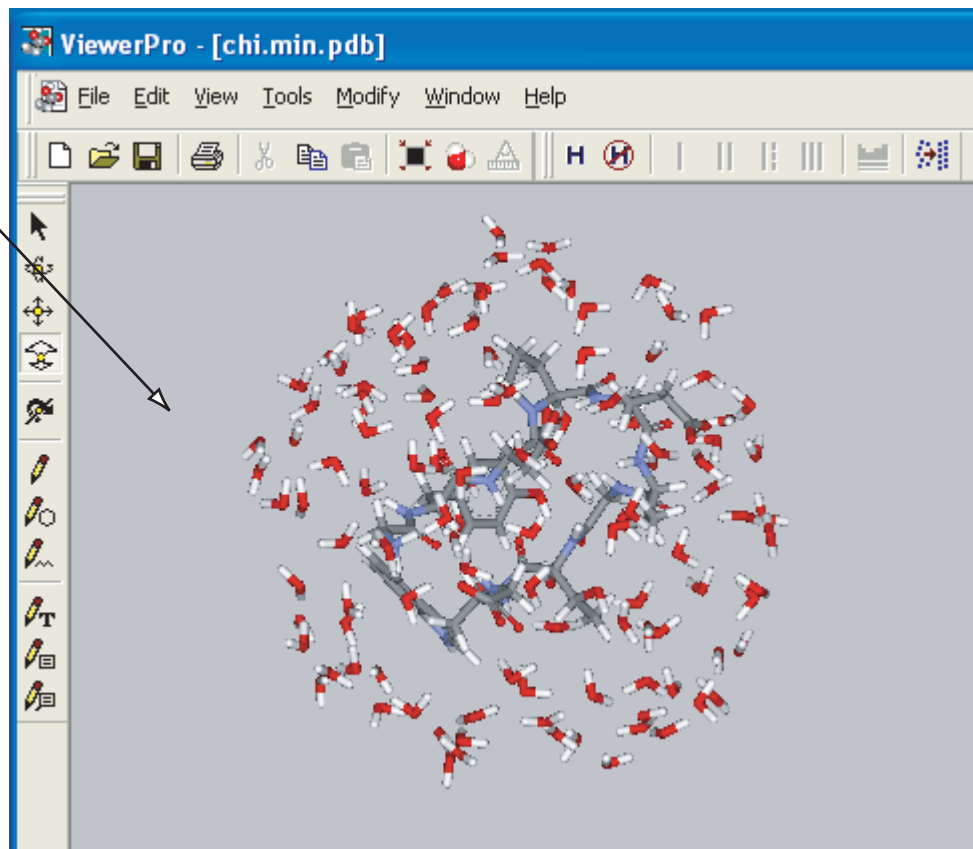
The image shows a screenshot of an SSH Secure Shell window titled "2:bono.ccr.buffalo.edu - U2 - SSH Secure Shell". The window displays a list of atoms from a PDB file. An arrow points from the text "The coordinates of TIP3P water molecules in the PDB file" to the line "ATOM 139 O WAT 11" in the table.

Atom	ID	Residue	Type	Chain	X	Y	Z
ATOM	133	CA	GLY	10	-1.229	-3.774	4.431
ATOM	134	2HA	GLY	10	-0.160	-3.949	4.312
ATOM	135	3HA	GLY	10	-1.387	-2.943	5.118
ATOM	136	C	GLY	10	-1.877	-5.031	5.014
ATOM	137	O	GLY	10	-1.289	-6.092	4.882
ATOM	138	OXT	GLY	10	-2.949	-4.912	5.584
TER							
ATOM	139	O	WAT	11	7.738	0.440	8.737
ATOM	140	H1	WAT	11	8.046	-0.115	8.021
ATOM	141	H2	WAT	11	6.808	0.575	8.555
TER							
ATOM	142	O	WAT	12	2.433	7.926	5.756
ATOM	143	H1	WAT	12	2.312	8.652	5.144
ATOM	144	H2	WAT	12	2.123	7.156	5.279

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5

MM dynamics of Chignolin in a sphere of water

Chignolin protein
surrounded by
water molecules



MM dynamics of Chignolin in a sphere of water

Technical details of minimization

2.bono.ccr.buffalo.edu - U2 - SSH Secure Shell

File Edit View Window Help

Quick Connect Profiles

```

2000 steps of minimization
&cntrl
    imin=1, ntmin=2, drms=0.20,
    ntb=0, cut=12,
    ntc=1, ntf=1,
    ntpr=100,
    maxcyc=2000,
/
~
~
~
~
~
~
~
"min.in" 8L, 138C

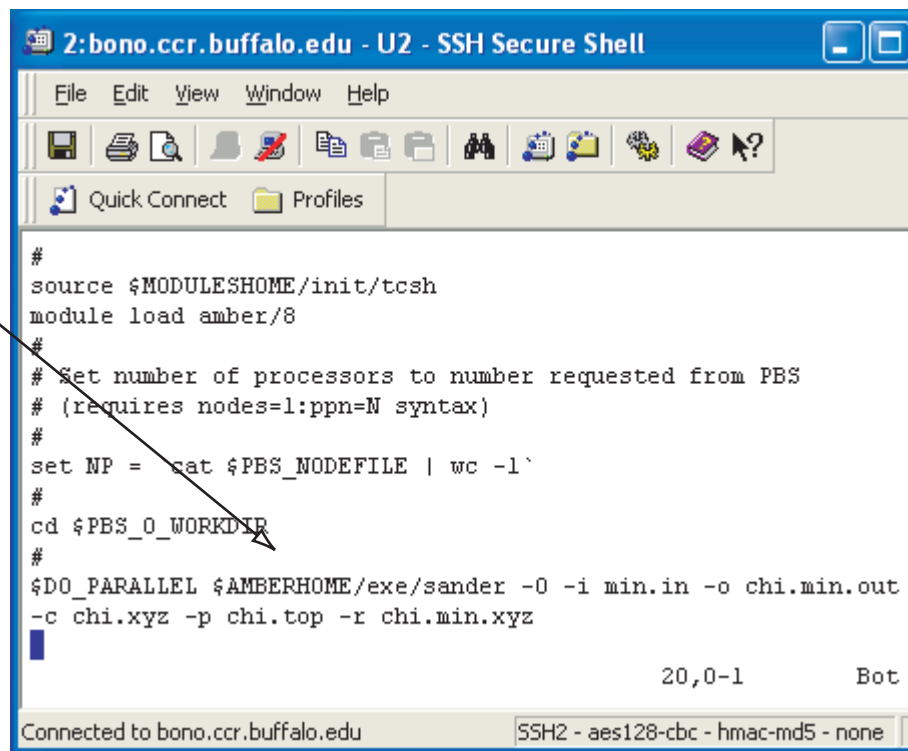
```

Connected to bono.ccr.buffalo.edu

SSH2 - aes128-cbc - hmac-md5

MM dynamics of Chignolin in a sphere of water

Technical details
of running
minimization



```
#
source $MODULESHOME/init/tcsh
module load amber/8
#
# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i min.in -o chi.min.out
-c chi.xyz -p chi.top -r chi.min.xyz
```

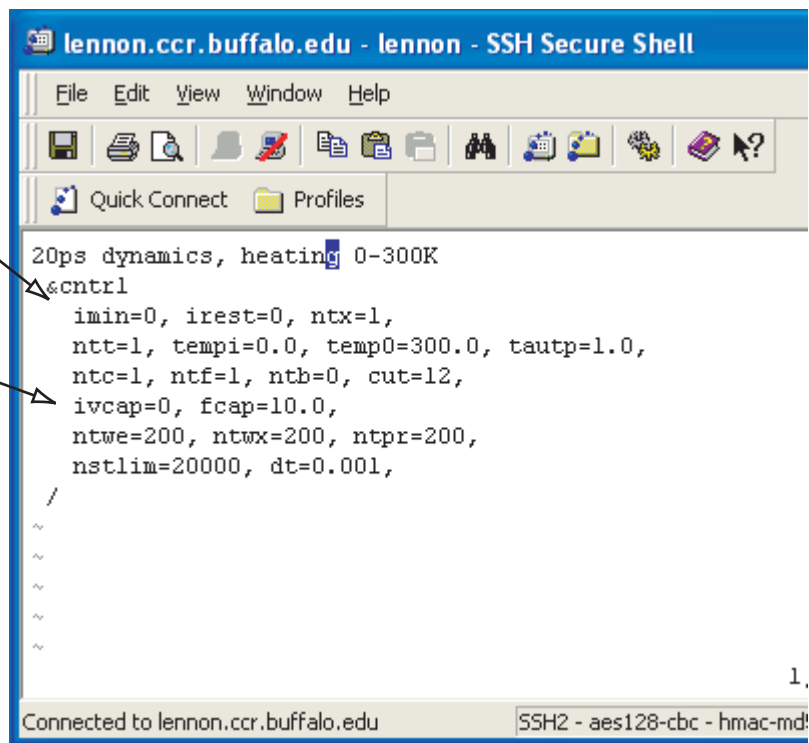
20,0-1 Bot

Connected to bono.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none

MM dynamics of Chignolin in a sphere of water

Technical details
of heating

Parameters of the
water sphere

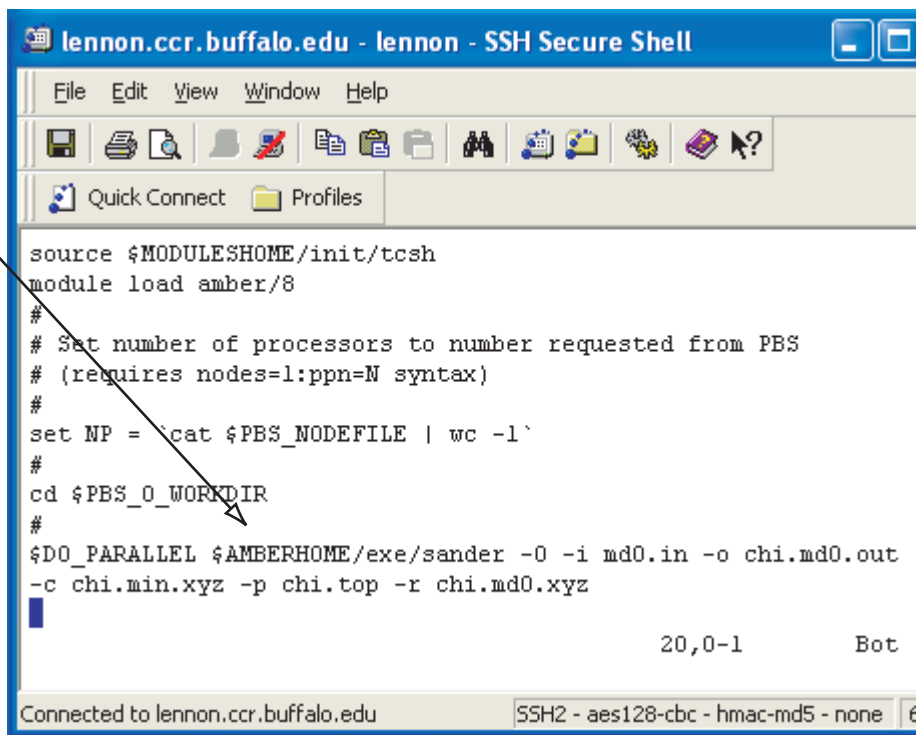


```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles
20ps dynamics, heating 0-300K
>ctrl
  imin=0, irest=0, ntx=1,
  ntt=1, tempi=0.0, temp0=300.0, tautp=1.0,
  ntc=1, ntf=1, ntb=0, cut=12,
  ivcap=0, fcap=10.0,
  ntwe=200, ntwx=200, ntpr=200,
  nstlim=20000, dt=0.001,
/
~
~
~
~
~
1,
```

Connected to lennon.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5

MM dynamics of Chignolin in a sphere of water

Technical details
of running
heating



```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Home, End, Up, Down, Left, Right, Search, Help]
Quick Connect Profiles

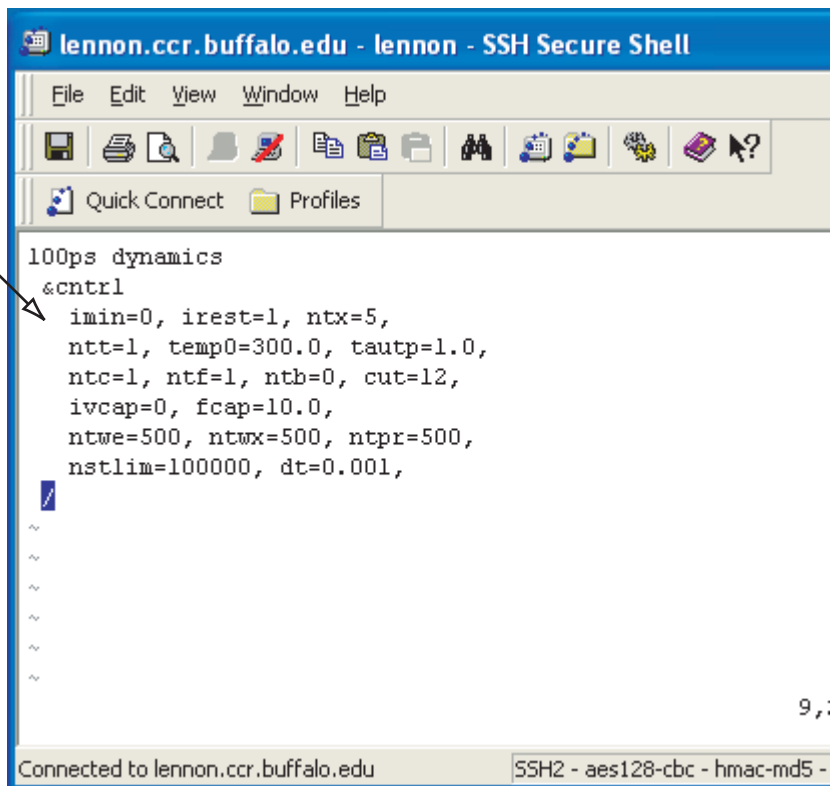
source $MODULESHOME/init/tcsh
module load amber/8
#
# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md0.in -o chi.md0.out
-c chi.min.xyz -p chi.top -r chi.md0.xyz

20,0-1 Bot

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none 6
```

MM dynamics of Chignolin in a sphere of water

Technical details
of dynamics



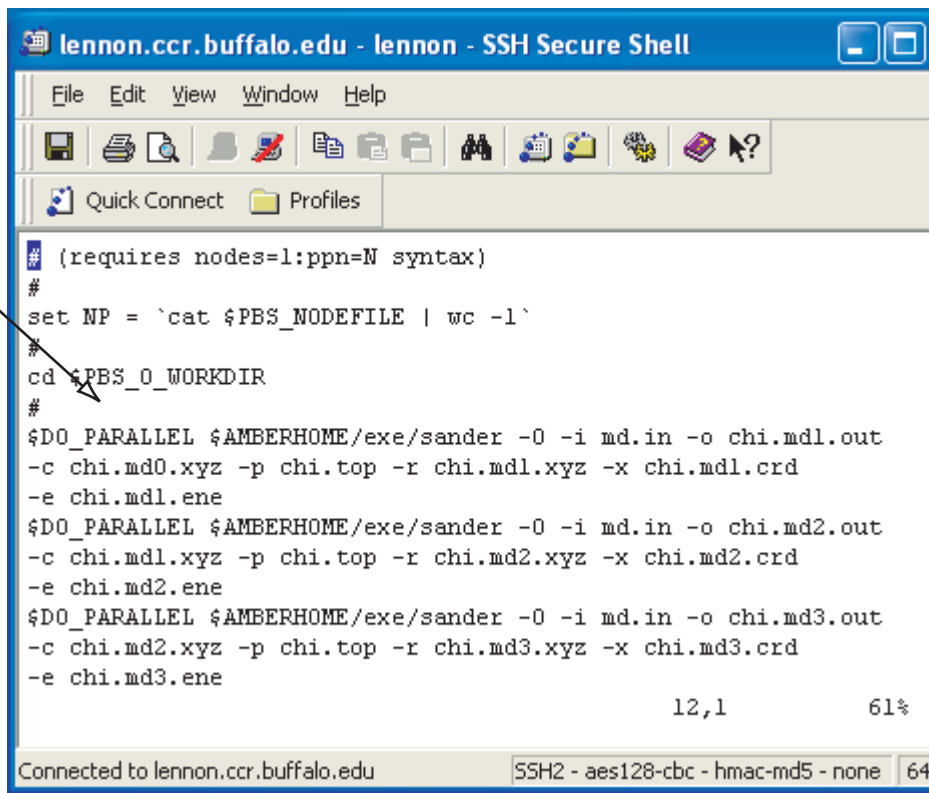
The screenshot shows an SSH Secure Shell window titled "lennon.ccr.buffalo.edu - lennon - SSH Secure Shell". The window has a menu bar (File, Edit, View, Window, Help) and a toolbar with icons for file operations and system functions. Below the toolbar is a "Quick Connect" section with a "Profiles" button. The main terminal area displays the following text:

```
100ps dynamics
&ctrl
  imin=0, irest=1, ntx=5,
  ntt=1, temp0=300.0, tautp=1.0,
  ntc=1, ntf=1, ntb=0, cut=12,
  ivcap=0, fcap=10.0,
  ntwe=500, ntwx=500, ntp=500,
  nstlim=100000, dt=0.001,
  /
~
~
~
~
~
~
```

At the bottom of the window, a status bar indicates "Connected to lennon.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-md5 -".

MM dynamics of Chignolin in a sphere of water

Technical details
of running
dynamics



```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Home, Up, Down, Left, Right, Search, Help]
Quick Connect Profiles

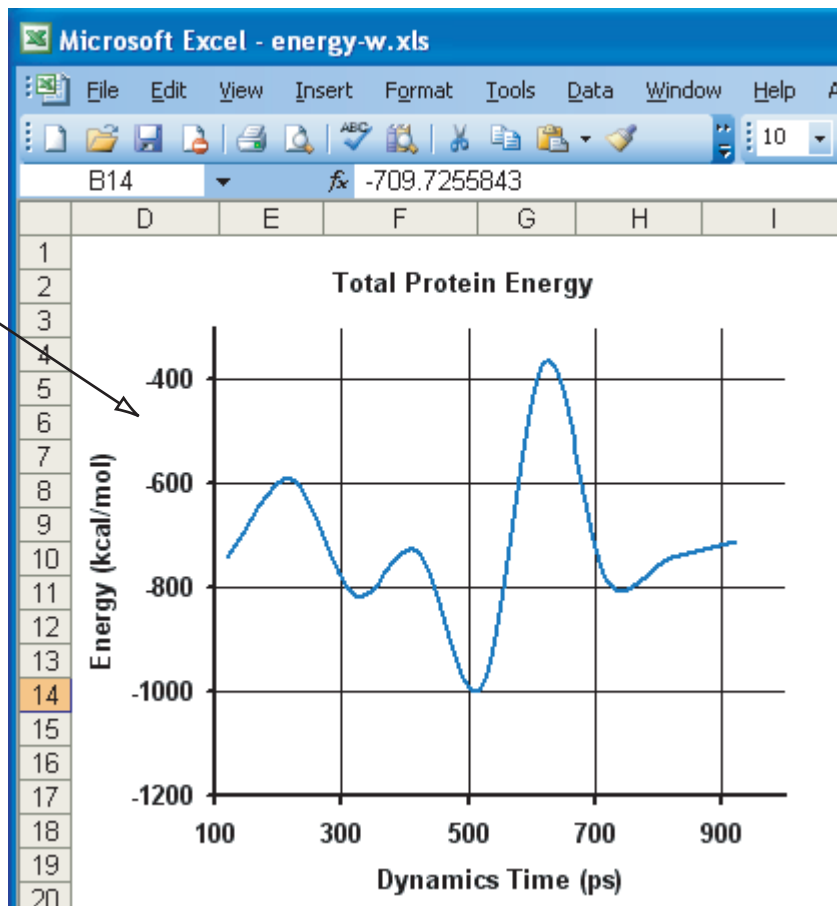
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.mdl.out
-c chi.md0.xyz -p chi.top -r chi.mdl.xyz -x chi.mdl.crd
-e chi.mdl.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md2.out
-c chi.mdl.xyz -p chi.top -r chi.md2.xyz -x chi.md2.crd
-e chi.md2.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o chi.md3.out
-c chi.md2.xyz -p chi.top -r chi.md3.xyz -x chi.md3.crd
-e chi.md3.ene

12,1 61%

Connected to lennon.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none 64
```

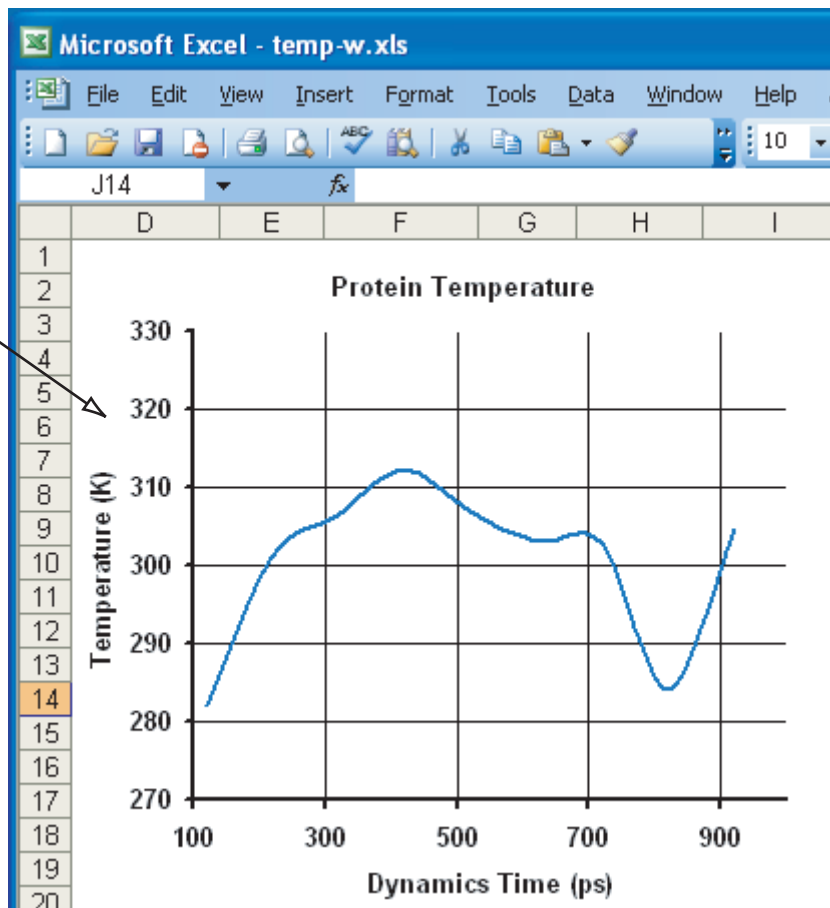
MM dynamics of Chignolin in a sphere of water

Total energy of
the protein after
dynamics in
water solution



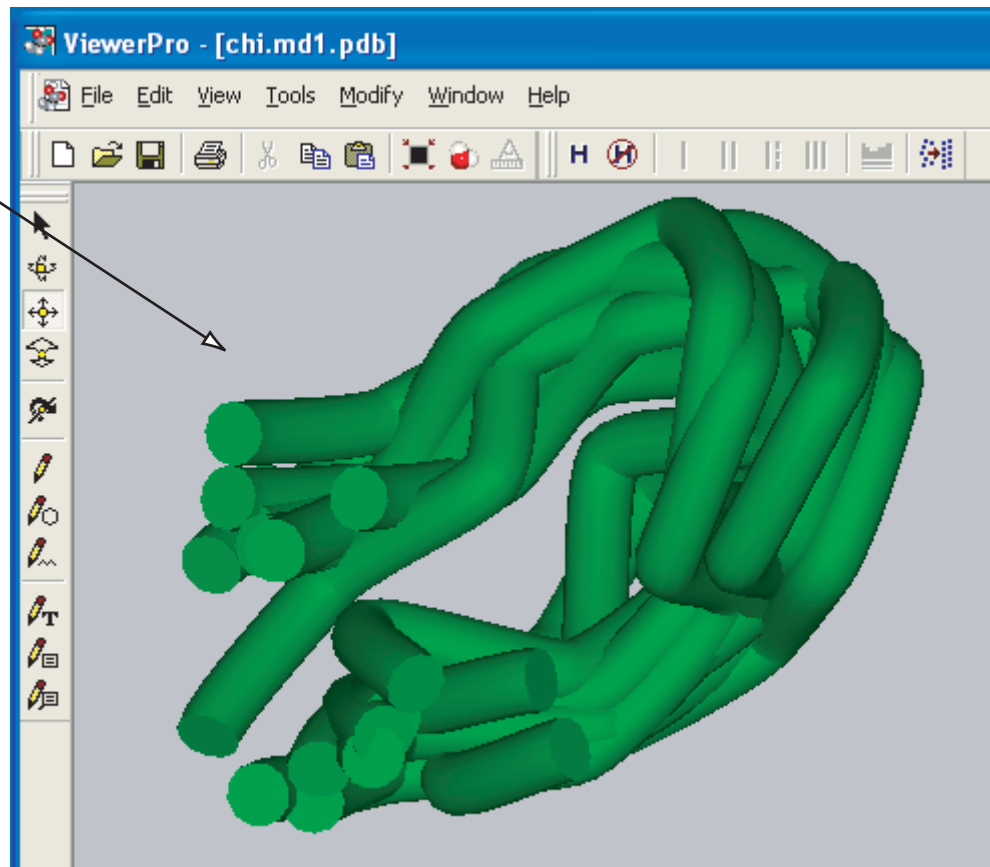
MM dynamics of Chignolin in a sphere of water

Temperature of
the protein after
dynamics in
water solution



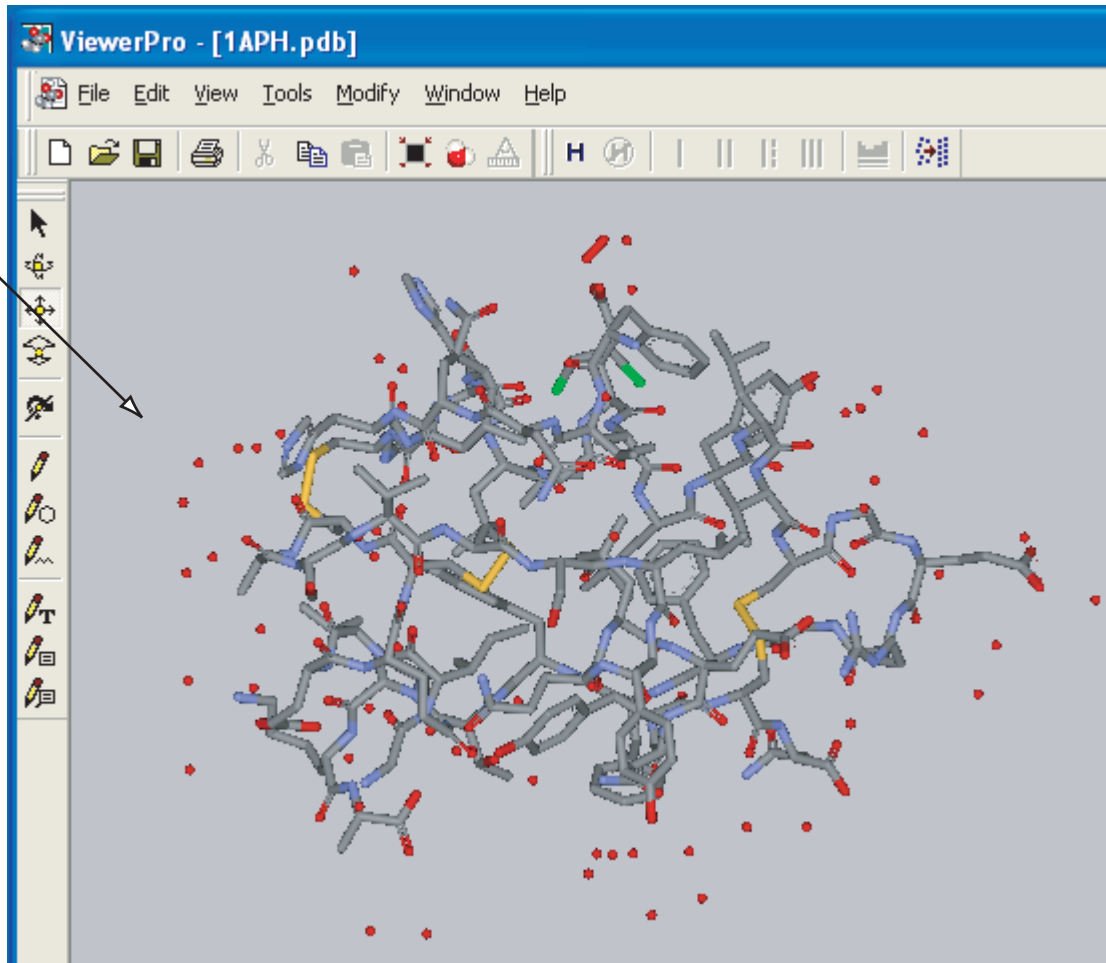
MM dynamics of Chignolin in a sphere of water

Superposition of 9
protein structure
obtained from MD
in water solution



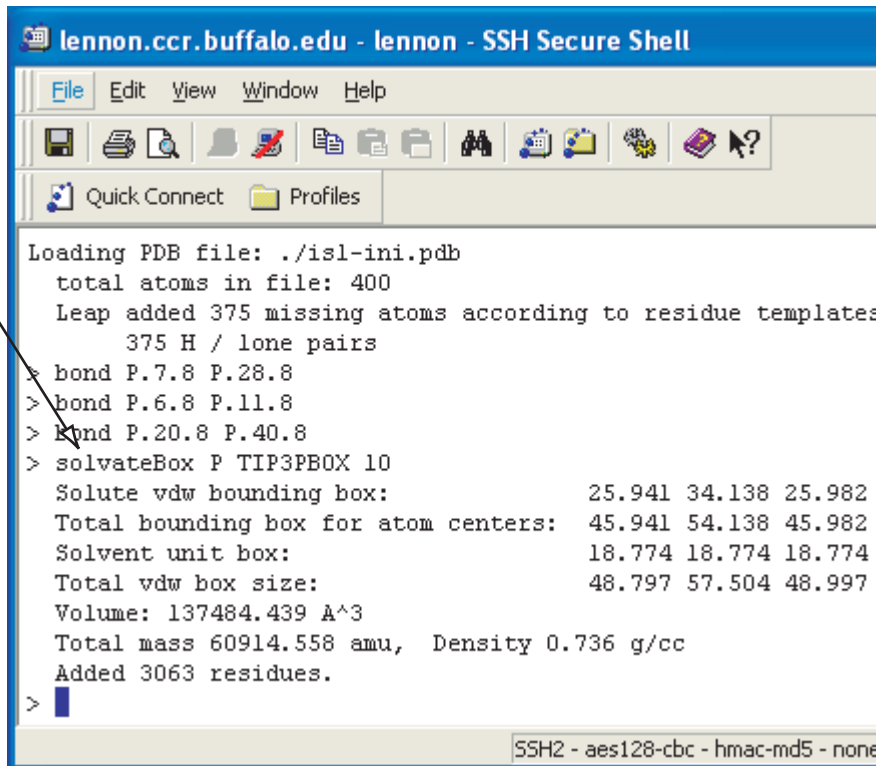
MM dynamics of Insulin in a periodic box of water

Experimental
PDB file of
Insuline



MM dynamics of Insulin in a periodic box of water

Solvating the protein
by a box of explicit
water molecules



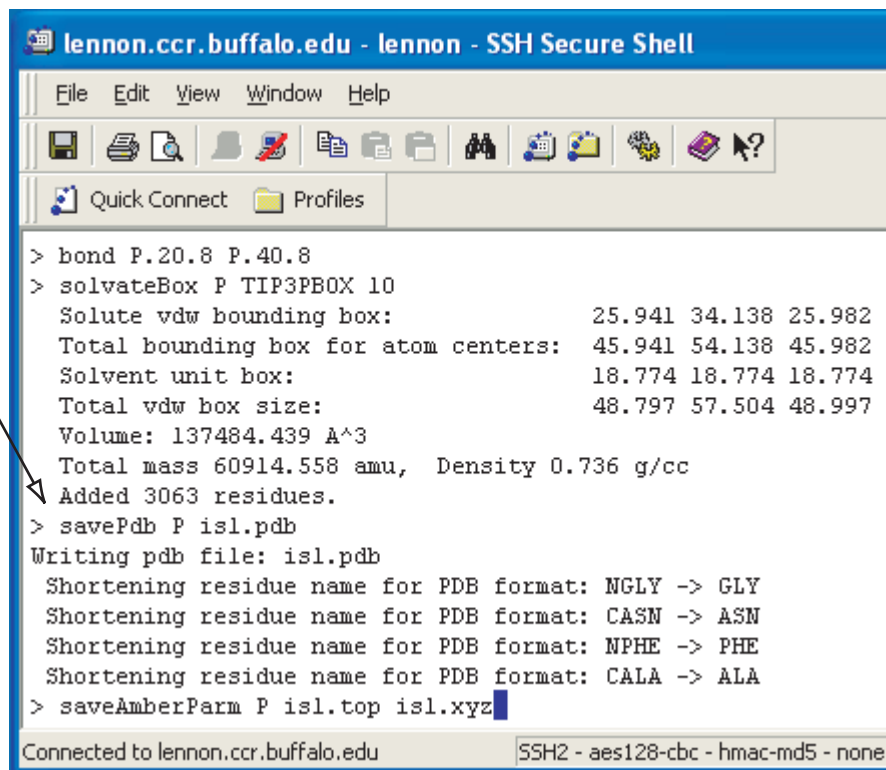
```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, Copy, Paste, Undo, Redo, Open, Save As, Print As, Run, Stop, Break, Help]
Quick Connect Profiles

Loading PDB file: ./isl-ini.pdb
total atoms in file: 400
Leap added 375 missing atoms according to residue templates
    375 H / lone pairs
> bond P.7.8 P.28.8
> bond P.6.8 P.11.8
> bond P.20.8 P.40.8
> solvateBox P TIP3PBOX 10
Solute vdw bounding box:                25.941 34.138 25.982
Total bounding box for atom centers:    45.941 54.138 45.982
Solvent unit box:                      18.774 18.774 18.774
Total vdw box size:                    48.797 57.504 48.997
Volume: 137484.439 A^3
Total mass 60914.558 amu, Density 0.736 g/cc
Added 3063 residues.
> 
```

SSH2 - aes128-cbc - hmac-md5 - none

MM dynamics of Insulin in a periodic box of water

Saving the PDB,
topology and
coordinates files



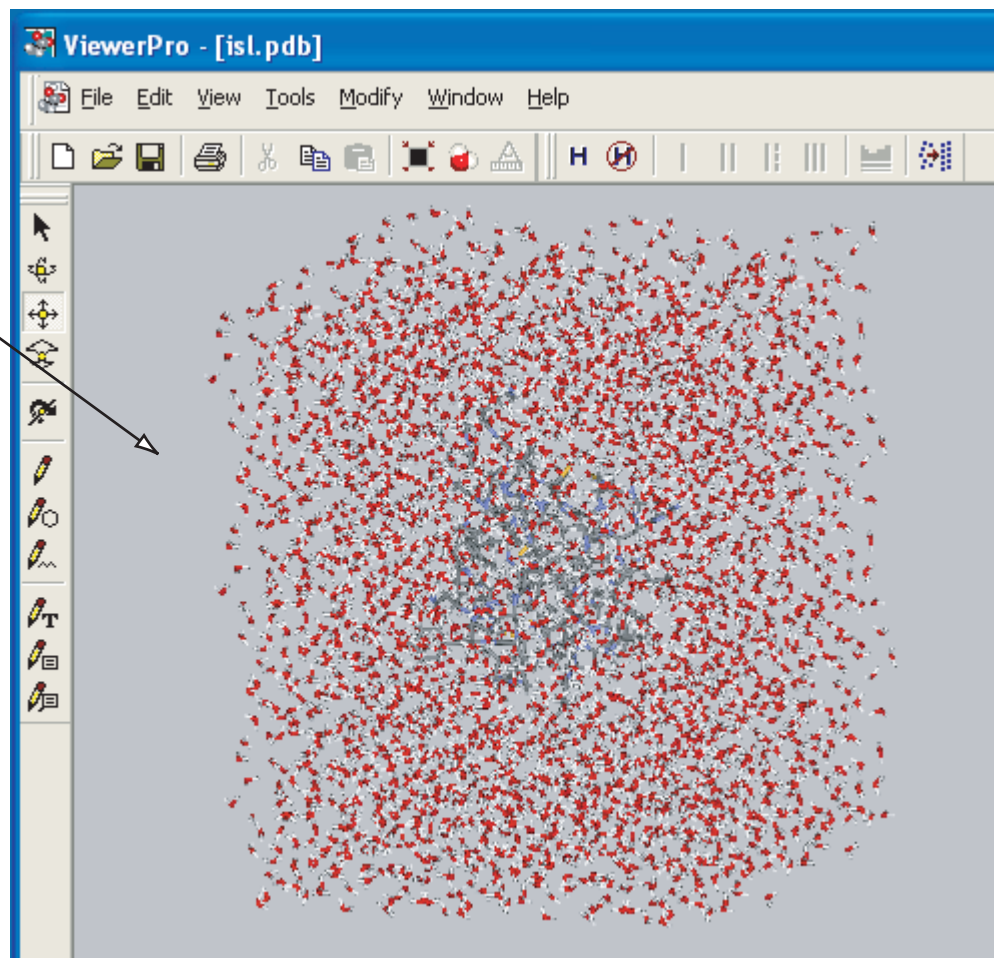
```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, etc.]
Quick Connect Profiles

> bond P.20.8 P.40.8
> solvateBox P TIP3PBOX 10
Solute vdw bounding box:           25.941 34.138 25.982
Total bounding box for atom centers: 45.941 54.138 45.982
Solvent unit box:                 18.774 18.774 18.774
Total vdw box size:               48.797 57.504 48.997
Volume: 137484.439 A^3
Total mass 60914.558 amu, Density 0.736 g/cc
Added 3063 residues.
> savePdb P isl.pdb
Writing pdb file: isl.pdb
Shortening residue name for PDB format: NGLY -> GLY
Shortening residue name for PDB format: CASN -> ASN
Shortening residue name for PDB format: NPHE -> PHE
Shortening residue name for PDB format: CALA -> ALA
> saveAmberParm P isl.top isl.xyz

Connected to lennon.ccr.buffalo.edu    SSH2 - aes128-cbc - hmac-md5 - none
```

MM dynamics of Insulin in a periodic box of water

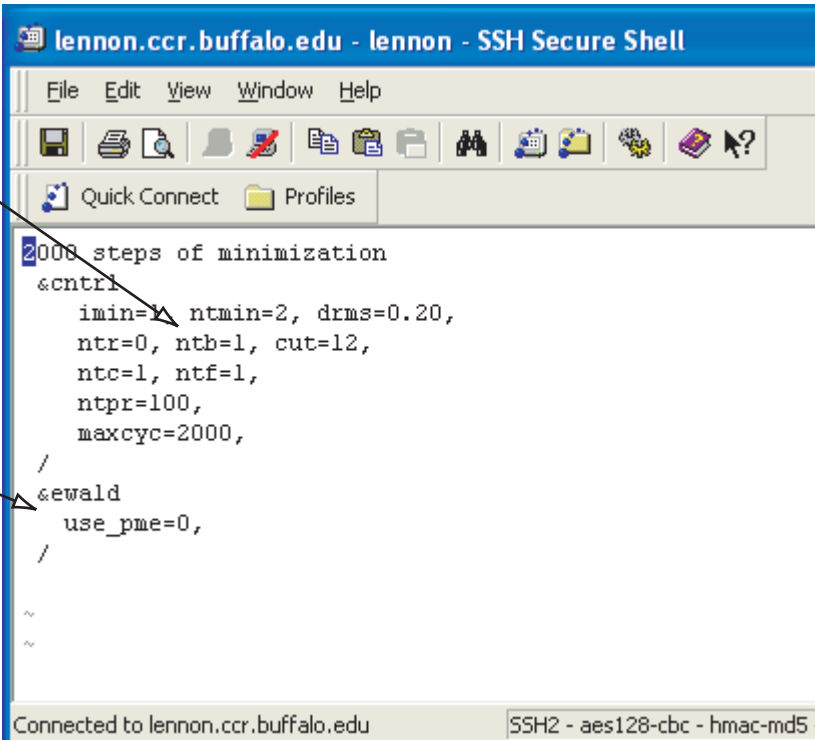
The PDB file of the protein in a periodic box of explicit water molecules



MM dynamics of Insulin in a periodic box of water

Technical details of
minimization in
constance volume

We are not using the
Particle Mesh Ewald
method



The screenshot shows an SSH terminal window titled "lennon.ccr.buffalo.edu - lennon - SSH Secure Shell". The window has a menu bar with "File", "Edit", "View", "Window", and "Help". Below the menu bar is a toolbar with various icons. The terminal content shows the output of a minimization process, including the number of steps and the parameters used. Two arrows from the text on the left point to specific lines in the terminal: one points to "2000 steps of minimization" and the other points to the "sewald" section.

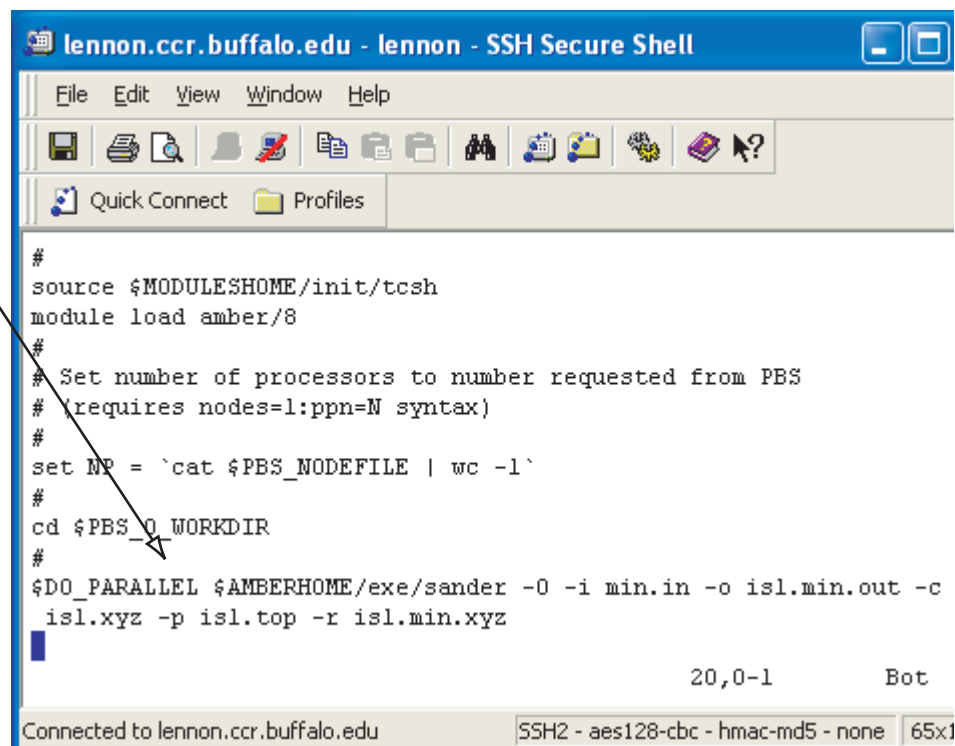
```
2000 steps of minimization
&cntrl
    imin=1, ntmin=2, drms=0.20,
    ntr=0, ntb=1, cut=12,
    ntc=1, ntf=1,
    ntp=100,
    maxcyc=2000,
/
sewald
    use_pme=0,
/
~
~
```

Connected to lennon.ccr.buffalo.edu

SSH2 - aes128-cbc - hmac-md5 -

MM dynamics of Insulin in a periodic box of water

Technical details
of running
minimization



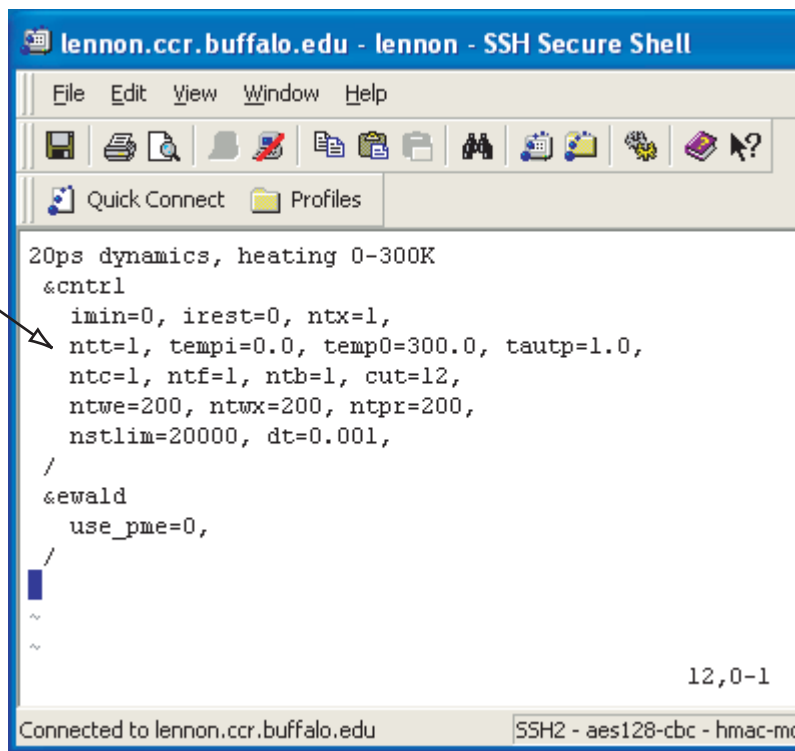
The screenshot shows an SSH terminal window titled "lennon.ccr.buffalo.edu - lennon - SSH Secure Shell". The terminal displays the following commands and output:

```
#
source $MODULESHOME/init/tcsh
module load amber/8
#
# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i min.in -o isl.min.out -c
isl.xyz -p isl.top -r isl.min.xyz
```

The terminal status bar at the bottom indicates "Connected to lennon.ccr.buffalo.edu", "SSH2 - aes128-cbc - hmac-md5 - none", and "65x1".

MM dynamics of Insulin in a periodic box of water

Technical details of
heating in constance
volume



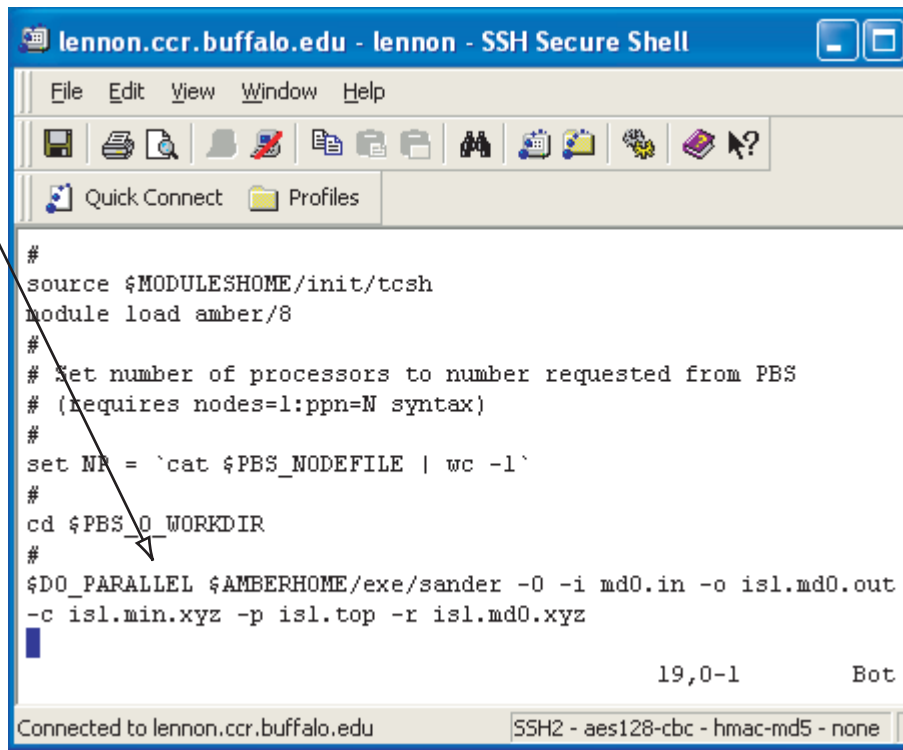
The screenshot shows an SSH terminal window titled "lennon.ccr.buffalo.edu - lennon - SSH Secure Shell". The terminal displays the following text:

```
20ps dynamics, heating 0-300K
&cntrl
  imin=0, irest=0, ntx=1,
  ntt=1, tempi=0.0, temp0=300.0, tautp=1.0,
  ntc=1, ntf=1, ntb=1, cut=12,
  ntwe=200, ntwx=200, ntpr=200,
  nstlim=20000, dt=0.001,
/
&ewald
  use_pme=0,
/
~
~
12,0-1
```

The terminal window includes a menu bar with "File", "Edit", "View", "Window", and "Help". Below the menu bar is a toolbar with various icons. At the bottom of the window, it shows "Connected to lennon.ccr.buffalo.edu" and "SSH2 - aes128-cbc - hmac-mc".

MM dynamics of Insulin in a periodic box of water

Technical details of
running heating



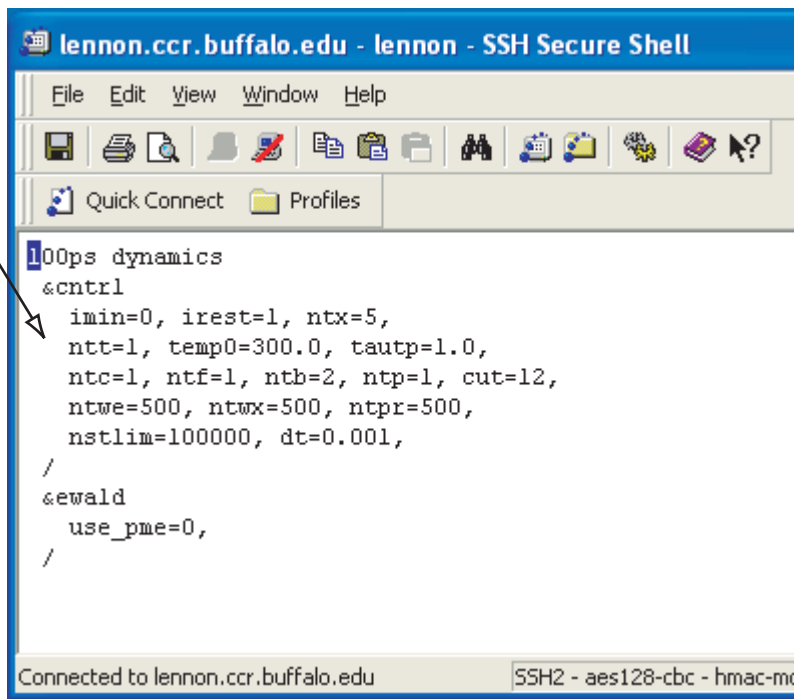
```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
[Icons: Save, Print, Find, etc.]
Quick Connect Profiles

#
source $MODULESHOME/init/tcsh
module load amber/8
#
# Set number of processors to number requested from PBS
# (requires nodes=1:ppn=N syntax)
#
set NP = `cat $PBS_NODEFILE | wc -l`
#
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md0.in -o isl.md0.out
-c isl.min.xyz -p isl.top -r isl.md0.xyz

19,0-1 Bot
Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5 - none
```

MM dynamics of Insulin in a periodic box of water

Technical details of
dynamics in constant
pressure



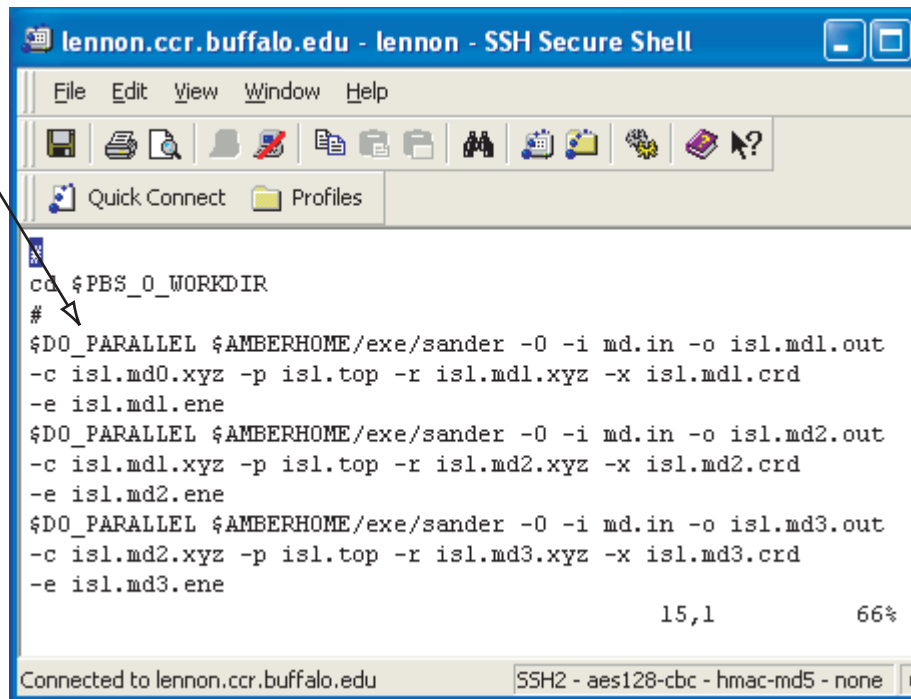
```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

100ps dynamics
&ctrl
imin=0, irest=1, ntx=5,
ntt=1, temp0=300.0, tautp=1.0,
ntc=1, ntf=1, ntb=2, ntp=1, cut=12,
ntwe=500, ntwx=500, ntp=500,
nstlim=100000, dt=0.001,
/
&ewald
use_pme=0,
/

Connected to lennon.ccr.buffalo.edu  SSH2 - aes128-cbc - hmac-md5
```


MM dynamics of Insulin in a periodic box of water

Technical details of
running dynamics



```
lennon.ccr.buffalo.edu - lennon - SSH Secure Shell
File Edit View Window Help
Quick Connect Profiles

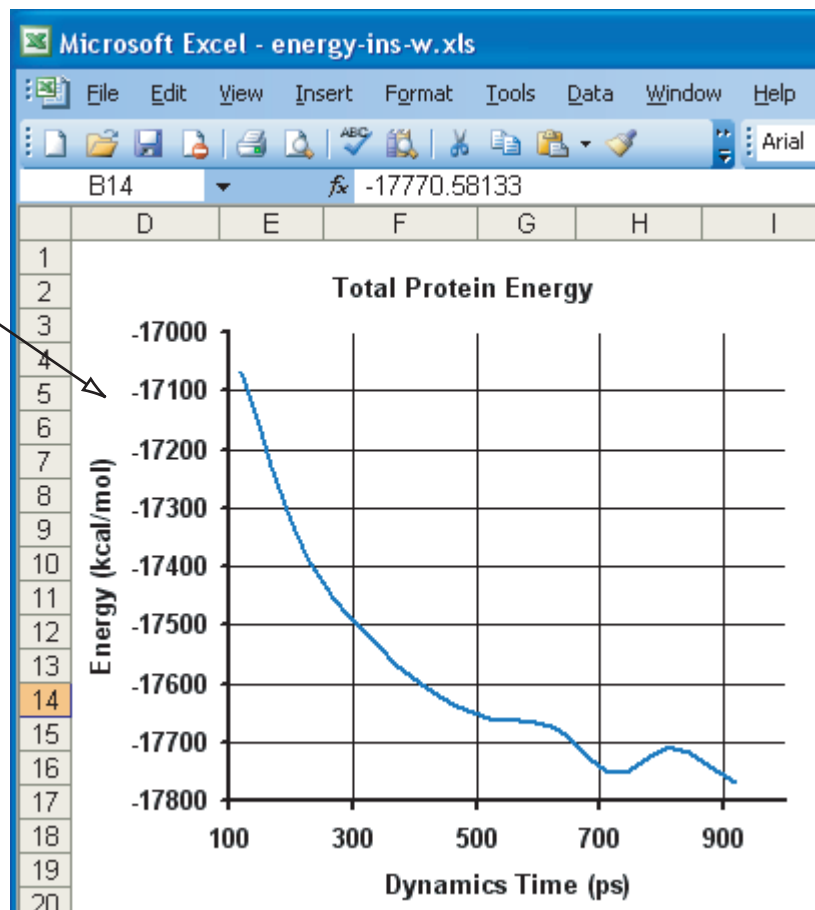
cd $PBS_O_WORKDIR
#
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o isl.mdl.out
-c isl.md0.xyz -p isl.top -r isl.mdl.xyz -x isl.mdl.crd
-e isl.mdl.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o isl.md2.out
-c isl.mdl.xyz -p isl.top -r isl.md2.xyz -x isl.md2.crd
-e isl.md2.ene
$DO_PARALLEL $AMBERHOME/exe/sander -O -i md.in -o isl.md3.out
-c isl.md2.xyz -p isl.top -r isl.md3.xyz -x isl.md3.crd
-e isl.md3.ene

15,1 66%

Connected to lennon.ccr.buffalo.edu SSH2 - aes128-cbc - hmac-md5 - none
```

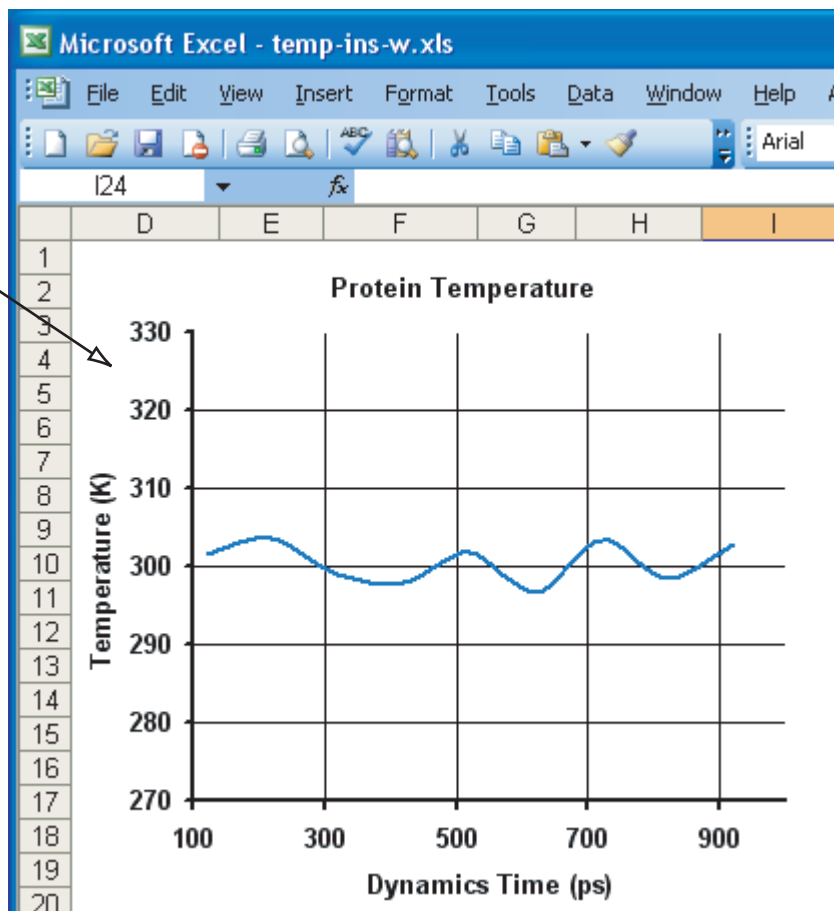
MM dynamics of Insulin in a periodic box of water

The energy of the protein after 1ns dynamics in water solution



MM dynamics of Insulin in a periodic box of water

The temperature of the protein after 1ns dynamics in water solution



MM dynamics of Insulin in a periodic box of water

Superposition of
9 protein
snapshots after
1ns dynamics in
water solution

