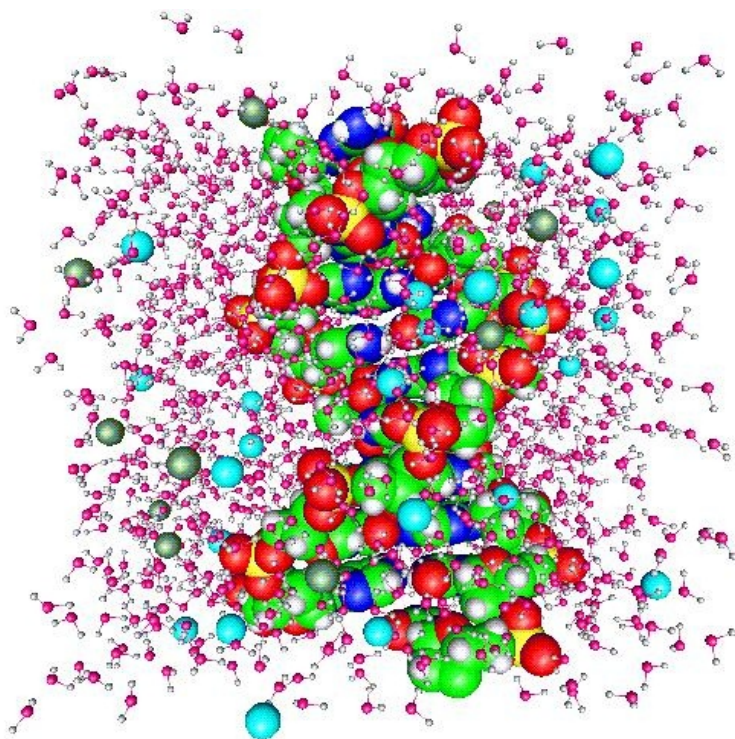


Visualization of molecular simulations

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Molecular dynamics: solution of Newtonian equations of motion in the molecular system

For each atom at each time:

$$v_i(t+1/2\Delta t) = v_i(t-1/2\Delta t) + F_i(\{x_j(t)\})/m_i \Delta t$$

$$x_i(t+\Delta t) = x_i(t) + v_i(t+1/2\Delta t) \Delta t$$

1998: MdynaMix - parallel scalable molecular dynamics for arbitrary molecular mixtures

http://www.fos.su.se/physical/sasha/md_prog.html

Current project: Interactive Visualisation

includes:

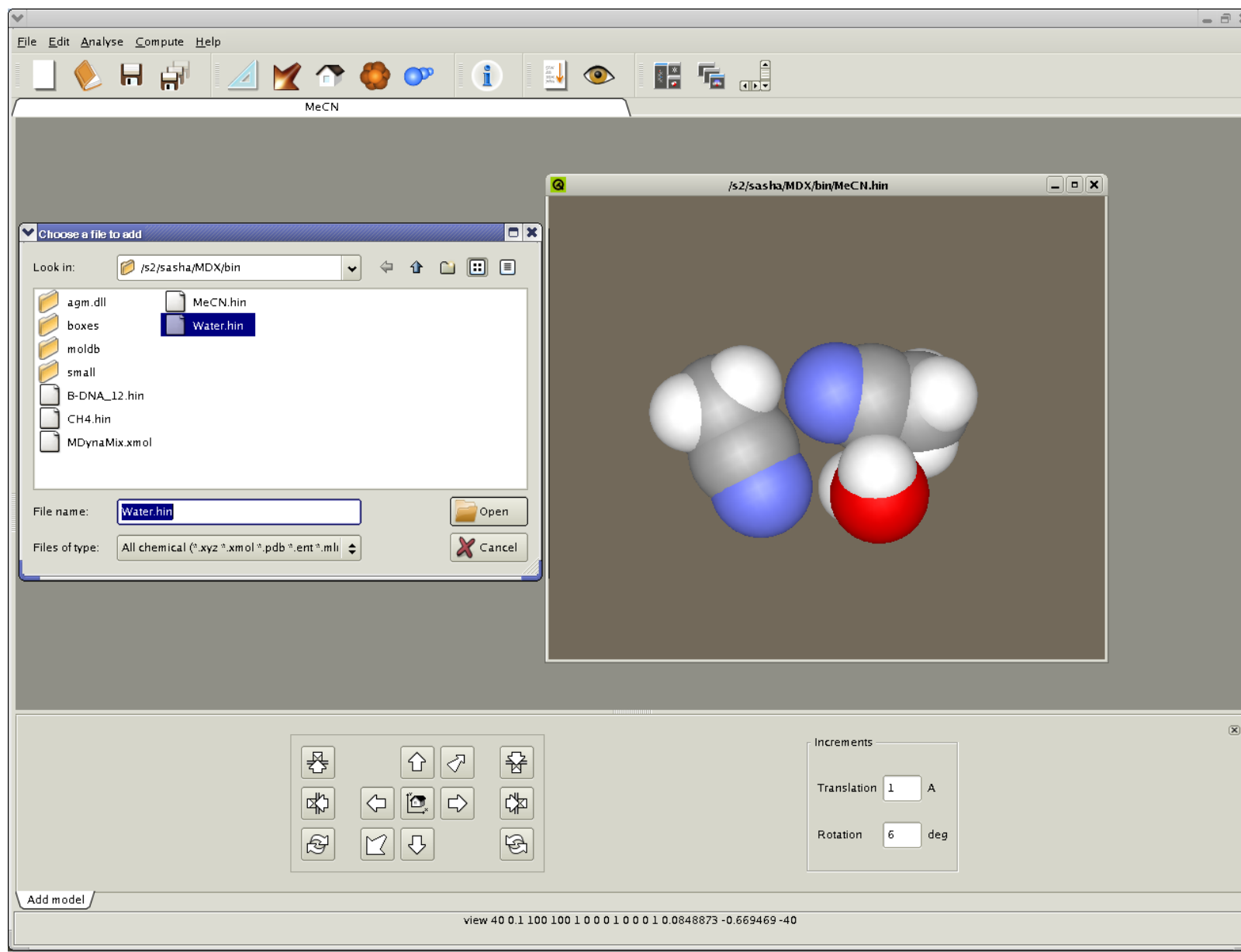
- initial preparing of molecular structures
- parameter (force field) association
- real-time visualization
- real-time analysis of result
- interactive: correction of simulation during the run

All these feature are implemented in MDX project

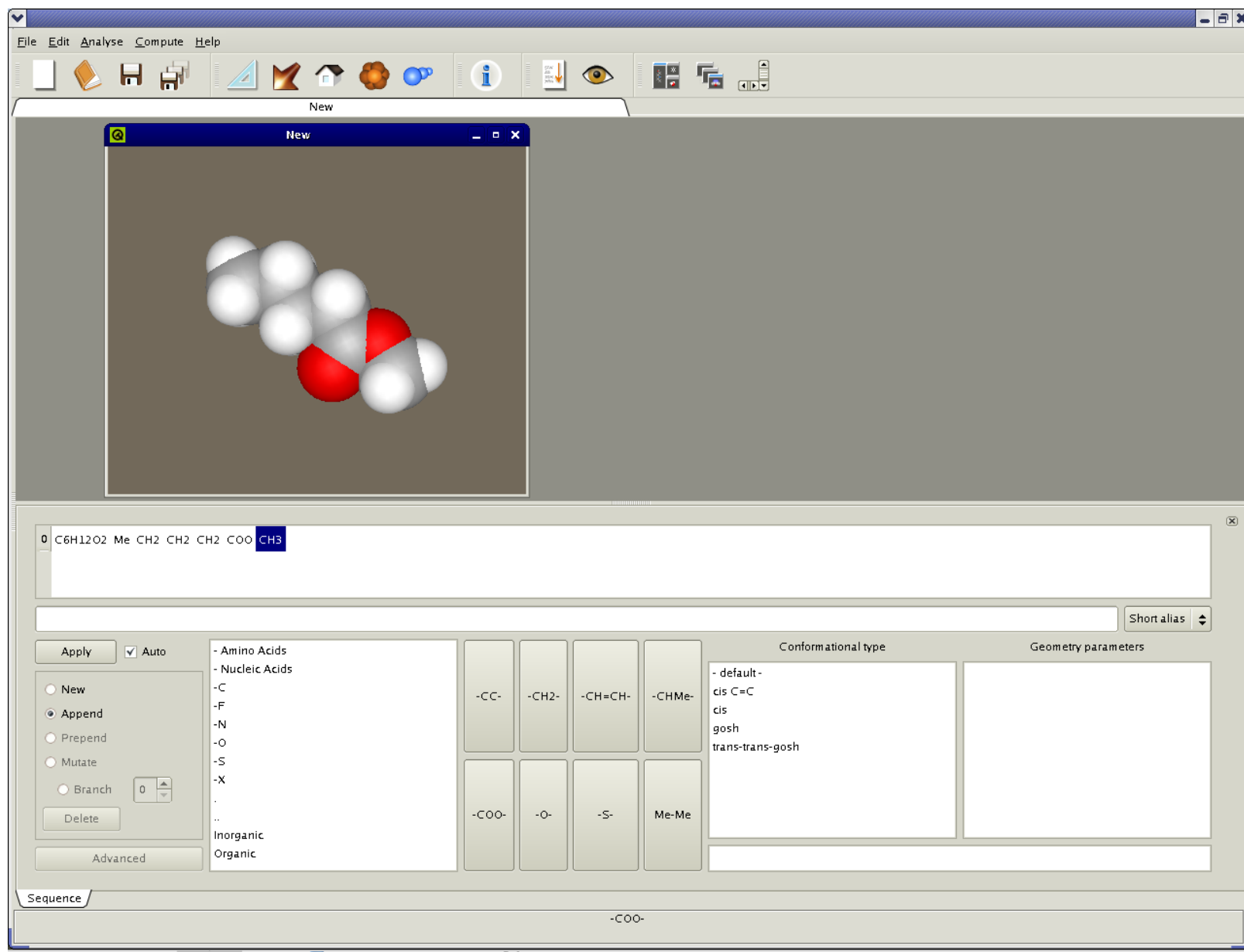
OS: Windows & Linux

Snapshots from the program:

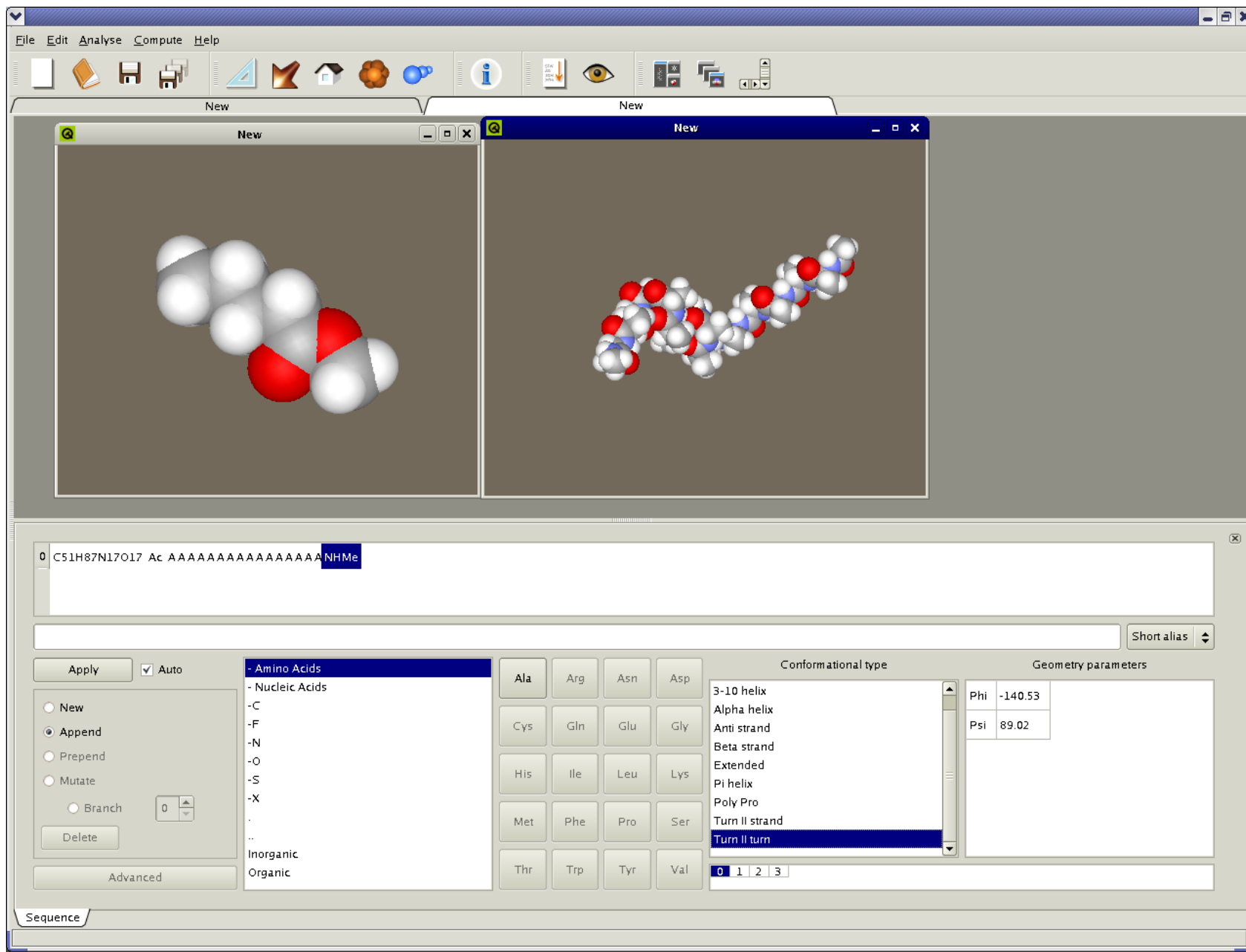
Building system from available structures



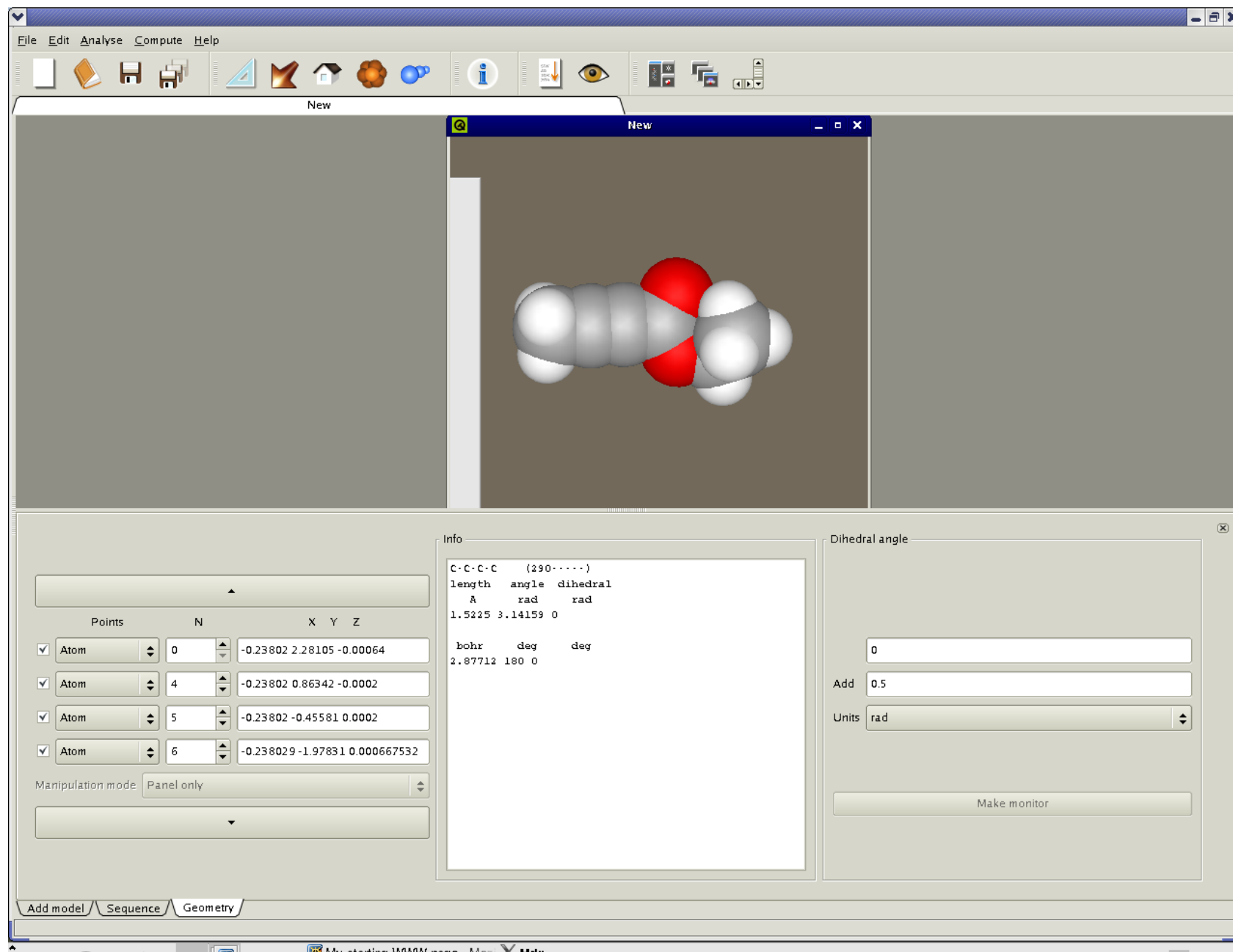
Building arbitrary molecular structures



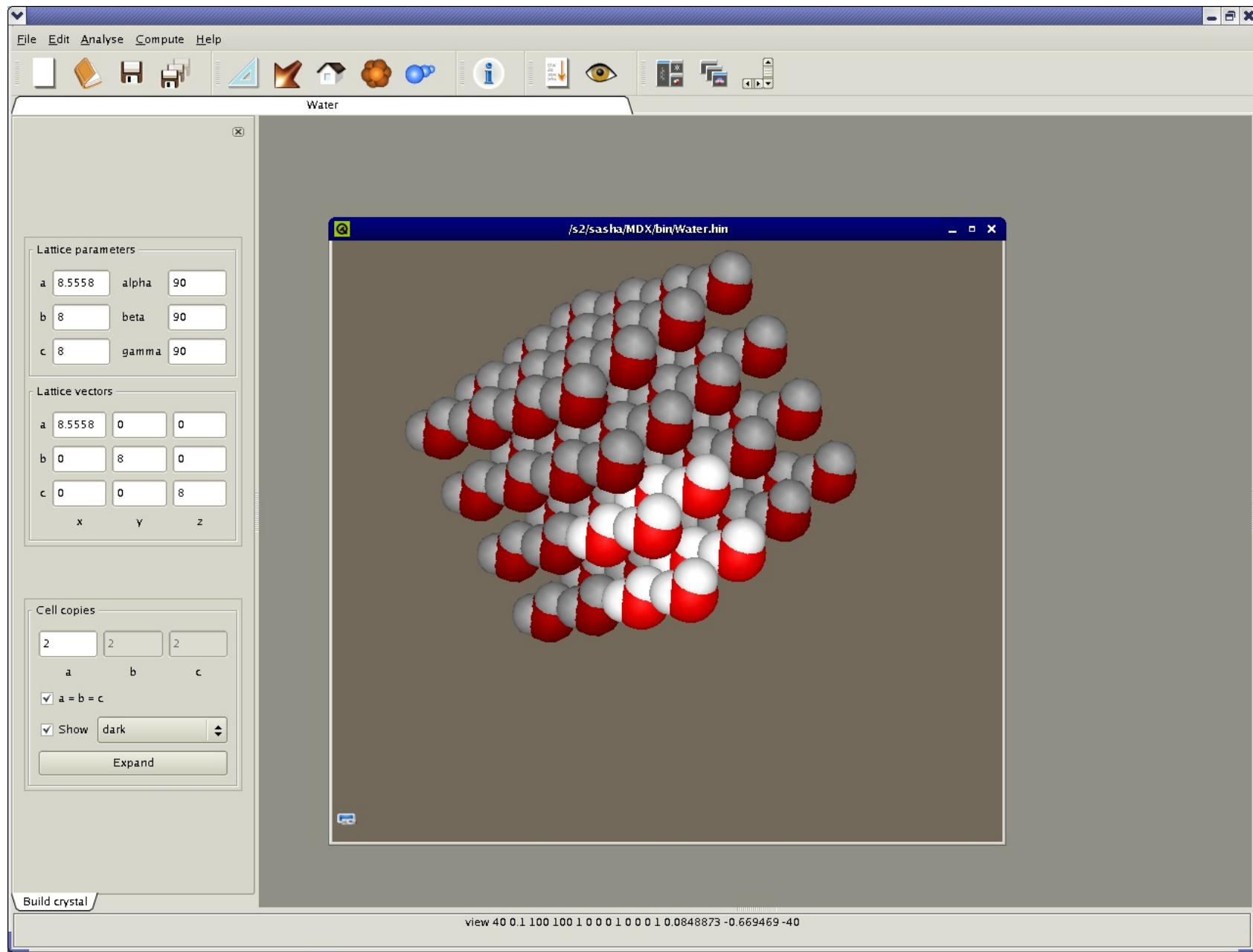
Building proteins



Geometry editing



Building a periodic system



Control of molecular dynamics run

Water

Output level: 5 Normal

Thermostat

☒ Nose 30 fs

☐ Simple scaling, delta 20 K

Barostat

700 fs

☐ Anisotropic NPT

Boundary Conditions

☐ Vacuum ☒ Box (A)

17.1116 16 16

☐ Manual ☒ From crystal ☐ Auto

Cutoff radius (A)

Lenard-Jones and Real-space 12

Fast forces 5

☐ Auto

Ewald

alpha*R 2.8 exp (m/s^{1/2}) 9 ☐ Auto

Dynamics

☒ cut large forces 0.1 ☐ constrained 0.0001

Steps

Long time step (fs) 2 Dump restart file after 500 steps

Small steps in long step 10 Check neighbours after 10 steps

Steps in series 1000 Final averaging after 1 series

Restart

☐ Read ☒ Dump ☐ Change temperature

Run

Stop

Tune

Start

Options

MDynaMix

cooling

heating

prepare

Intention	Method	Length	T	P	Comment
Initial conditions	MDynaMix	0 steps	10 K		
Equilibration	MDynaMix	0.2 ps	10 K		
Equilibration	MDynaMix	2 ps	25 deg		
Equilibration	MDynaMix	20 ps	25 deg		
Equilibration	MDynaMix	20 ps	25 deg	100 atm	
Pause		10 sec			Time in seconds
Equilibration	MDynaMix	100 ps	25 deg	1 atm	
Production	MDynaMix	100 ps	25 deg	1 atm	

Build crystal m.DynaMix

Protocol

view 40 0.1 100 100 1 0 0 1 0 0 0 1 0.0848873 -0.669469 -40

Monitoring physical quantities

