The following gives a brief description on LIBMOL (or other name) package

(1) Location of Program Codes:

The source codes and required tables are in a repository located at “compx: /home/share/libmol-repo/, and can be checked out by bazaar commands

(2) Components of Program Codes:

After check out, the root directory should be LIBMOL, under which the following sub-directories and files should exist, include/, src/, lib/, main.cpp, Makefile.

(3) Installation:

(a) Type

make clean

make

in the root directory where Makefile resides.

If the compilation is successful, there should be a binary file “libmol” under the subdirectory bin/

(b) Recursively copy all data tables and subdirectories (such as allOrgAngleTables/) under the sub-directory lib/ into $CLIBD\_MON (you should have CCP4 suite installed). Note: do not copy sub-directory lib/ itself to $CLIBD\_MON. Those tables and subdirectories (such as allOrgAngleTables/) should be directly under $CLIBD\_MON.

(4) Run the program:

Two mostly used commands running the program are

1. ……./LIBMOL/bin/libmol –c your\_mmcif\_file –r your\_3\_letter\_ligand\_code –o your\_output\_dictionary\_file
2. ……/ LIBMOL/bin/libmol –s your\_mol\_or\_sdf\_file –r your\_3\_letter\_ligand\_code –o your\_output\_dictionary\_file

where,

“your\_mmcif\_file” is a input ligand structural file of mm\_cif format, just like those cif files for currently CCP4 dictionary.

“your\_mol\_or\_sdf\_file” is an input ligand structural file of MOL/SDF format.

“your\_3\_letter\_ligand\_code” is any 3 letter code you would like to use for the ligand.

(5) Program output:

The successfully completion of above two commands will produces at least two files.

1. “your\_output\_dictionary\_file” is the library file of mm\_cif format, just as those \*.lib files generated by “libcheck”
2. a file of PDB format contain ligand geometry optimized based on the values of bonds, bond angles, torsions, etc given in “your\_output\_dictionary\_file”. It shares the same name root with “your\_output\_dictionary\_file”, but with extension “.pdb”