Manual for Walker's Extension to ROD

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1 Introduction

An extension to ROD has been written to display the structure being fitted in the molecular graphics package RasMol[1]. RasMol allows visualisation of the structure in 3D.

Working with molecules rather than atoms increases the complexity of the structure analysis considerably. An important control, in order to check that models are programmed correctly, and that refinements make sense, is graphic visualization of structures.

For this purpose we have interfaced ROD with the freeware package RasMol. At this level, it is possible to write a RasMol xyz file of the bulk and surface model. Another important tool is distance checking. The distance check routine calculates the distance of each pair of atoms and produces a warning if two atoms are unphysically close. Both tools help to ensure that refined models are physically sound.

2 RasMol extensions to ROD

2.1 Quick Start

RasMol version 2.6 or greater for UNIX/Linux is required. For downloading the software or obtaining more information about installing and running it, see the RasMol website[2]]. There is a version for Windows but it does not seem to work with ROD (more precisely, it does not seem to enable BSD style socket communications).

To get started, do the following:

1. Start `rasmol` in the same directory as `rod`.

   If `rasmol` displays the message

   ```
   Unable to find RasMol help file!
   ```

   you can set the environment variable `RASMOLPATH` to the directory with the help file `rasmol.hlp` Note that this is not a critical error – you can use `rasmol` without the help file.

2. Run the following commands in `rod`:

   ROD> *extensions walker activate yes*

   ROD> *extensions walker rasmol display*

2.2   Description of extension (ext.wal)

2.3   ext.wal

2.3.1   ext.wal.set

ext.wal.set.rasmol

filename   the filename of the temporary xyz structure file
host   the machine RasMol is run on (default: localhost)
port   the port RasMol is listening on (default: 21069)

ext.wal.set.xyz

xcells   the number of unit cells in x direction
ycells   the number of unit cells in y direction

2.3.2   ext.wal.ras

display   send structure to RasMol
command send a command directly to RasMol

2.4   Details of implementation

ROD saves the structure to a temporary xyz file (defined by the `ext.wal.set.rasmol.filename` option), and then communicates with RasMol using BSD style sockets. Usually, RasMol would be run on the same machine as ROD, and `host` would therefore be set to `localhost`. It is possible however for ROD and RasMol to run on different machines. At present it is necessary that ROD and RasMol share a filesystem to store the structure file.

The `ext.wal.rasmol.command` option makes it possible to send a RasMol command from within ROD. For example it would be possible to change atom colour from within ROD.

2.5   Further work

It is only possible for one RasMol process to listen on the standard port. If someone else gets there first, then you will have to work out how to get RasMol to listen on a different port so ROD can talk to it.

Ideally it would not be necessary to save the structure to a temporary file, but just pass the structure down the socket connection. This would make running ROD on one machine and RasMol on another much simpler. It is currently not possible to do this with RasMol.

3   Bibliography

[1] Roger Sayle and E. James Milner-White. Rasmol: Biomolecular graphics for all. Trends in
    Biochemical Sciences (TIBS), 20(9):374, September 1995

[2] www.OpenRasMol.org