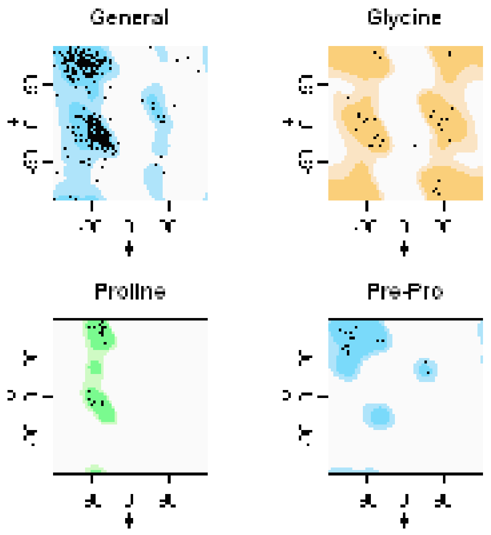
Drawing Ramachandran (phi/psi) plots for Proteins

These pages shows how to use R to draw a protein backbone's psi/phi torsion angles (ϕ,ψ) from a supplied file as a scatter plot overlayed on a filled contour plot showing the favoured and allowed regions, for example:



This R example does not read PDB files to calculate the (ϕ,ψ) angles directly - you have to supply them as an input file. For example, this tab separated variable file which I created using Python from PDB file 1HMP.

The code also relies on supplied background distributions to draw its filled contour plot - these datafiles are from Lovell *et al.* 2003 (see references). The colour scheme used is that of their online tool RAMPAGE (see other tools/programs for Ramachandran Plots), which produces even nicer images.

Loading the Phi/Psi angles for your protein

My code assumes you will have an input file where each line contains one (ϕ,ψ) angle pair (between -180 and 180 degrees) with the associated "Ramachandran Type" - i.e. Glycine, Proline, Pre-Proline or General.

The example input file (1HMP_mmtk.tsv, tab separated variable file created in python) looks like this:

```
1HMP:chain0:Pro5        -92.920842      12.941312       Proline
1HMP:chain0:Gly6        65.796887       -162.229709     Glycine
1HMP:chain0:Val7        -81.132882      121.413022      General
...
1HMP:chain1:Lys216      -168.783085     -116.244225     General
```

We can read this into R using the first column as the row name with one command:

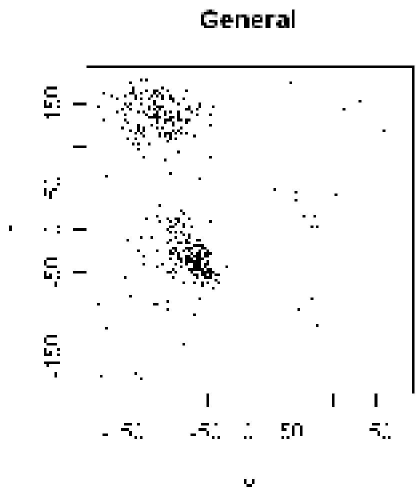
```
scatter.data <- read.table("1HMP_mmtk.tsv", header=FALSE, comment.char="", row.names=1,
colClasses=c("character","numeric","numeric","factor"), col.names=c("name","phi","psi","type"))
```

Its then very easy to filter this to get just the "Glycine" pairs for example:

```
> scatter.data[which(scatter.data[,"type"]=="Glycine"),"phi"]
 [1]   65.79681   79.01638  -54.12254  -56.43478   85.66384
 [6] -109.14374 -170.14536   23.78637 -106.75558 -115.52499
[11]   61.59938   95.28372   68.70101  -75.43935  103.26283
[16]  -68.65742   81.68372   71.33807  -69.08505  -66.91649
[21]  101.40772  107.48315 -131.43212  -67.83675  -95.88951
[26]  -86.20875   86.26477   87.74782   79.22726  -83.67855
[31]  103.86635  -55.16140
> scatter.data[which(scatter.data[,"type"]=="Glycine"),"psi"]
 [1] -162.229709 -136.703332  -38.858768  151.516345    9.247443
 [6]   11.702525  178.494853  -52.570408   22.092137  -17.593558
[11]   14.708826    6.490617   24.583907  -53.403879  159.510235
[16]  -29.319241 -164.401138 -155.176242  -32.708979  165.832486
[21]  -39.933404   32.899630   56.793570    6.169893    1.919425
[26]    5.175914  -17.154791  -15.588814   -4.129135  -52.845410
[31]  163.277791  -51.899098
```

Using R's plot command creating a simple scatter plot is then very easy:

```
> scatter.psi <- scatter.data[which(scatter.data[,"type"]=="General"),"psi"]
> scatter.phi <- scatter.data[which(scatter.data[,"type"]=="General"),"phi"]
> par(pty="s")
> plot(x=scatter.phi, y=scatter.psi, xlim=c(-180,180), ylim=c(-180,180), main="General", pch=20, xlab=expression(phi),
ylab=expression(psi), pch=20, cex=0.1, asp=1.0)
```



Note that we used `xlab=expression(phi)` to get the Greek letter ϕ as the x-axis label. The option `pch=20` gives dots (rather than the default of circles) for each datapoint, and `cex=0.1` makes them smaller than by default. Finally `asp=1.0` asks for an aspect ratio of one, and `par(pty="s")` requested a square plotting area.

Loading the Phi/Psi density profile

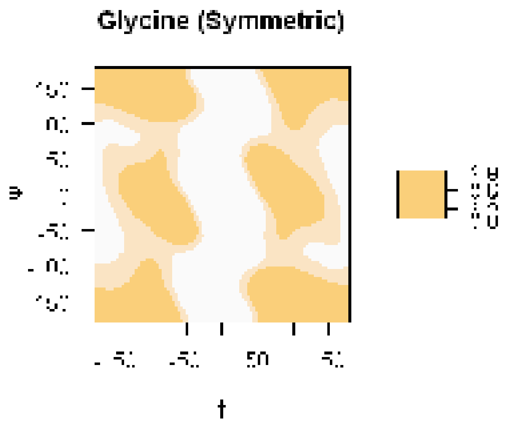
The following code is written to load the `rama500-*.data` files from Lovell et al. 2003 (see references, and downloads). For example, their file `rama500-general.data` looks like this:

```
# Table name/description: "Top500 General case (not Gly, Pro, or pre-Pro) B<30"
# Number of dimensions: 2
# For each dimension, 1 to 2: lower_bound  upper_bound  number_of_bins  wrapping
#   x1: -180.0 180.0 180 true
#   x2: -180.0 180.0 180 true
# List of table coordinates and values. (Value is last number on each line.)
-179.0 -179.0 0.00782923406455425
-179.0 -177.0 0.00641357067237856
-179.0 -175.0 0.005231799492823202
-179.0 -173.0 0.0042346800060073368
...
179.0 179.0 0.006881355097619223
```

I wrote an R function to load this data format, and turn it into an array suitable for use with R's contour functions (see downloads). It assumes that the grid is 180 by 180 in size (2 degrees per bin) with the grid points (mid points) at -179, -177, ..., to 179 degrees. For reasons of speed, it also make a big assumption about the order that the data will be found in...

Having loaded the data, you can draw it using the `contour` or `filled.contour` functions:

```
> par(pty="s")
> filled.contour(x=mid.points, y=mid.points, z=grid, levels=c(0,0.002,0.02,1), col=c("#FFFFFF","#FFE8C5","#FFCC7F"),
main="Glycine (Symmetric)", asp=1.0, xlab=expression(phi), ylab=expression(psi))
```



The thresholds are from the original reference, and the glycine colours are as used in RAMPAGE.

As before, we ensured a square plot area with `par(pty="s")` and setting the aspect ratio to one (`asp=1.0`). As far as I can tell, there is no way to turn off the key (which is worse the useless in this case), but all is not lost...

Combining Scatter & Contour Plots

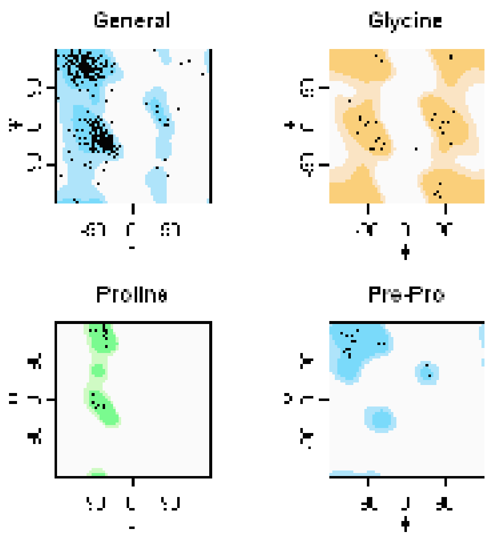
One of the nice things about R is that you can look at the source code to most of the built in functions - just try typing `filled.contour` at the R command prompt. I started with a copy of this code, removed the bits to draw the key, and added code to overlay a scatter plot to make my own function, `ramachandran.plot` (see downloads).

This preample code setups the filenames, thresholds, and colours for the four different plots:

```
mid.points <- seq(-179,179,2)

grid.filenames <- c(General="rama500-general.data",
                    Glycine="rama500-gly-sym.data",
                    Proline="rama500-pro.data",
                    Pre.Pro="rama500-prepro.data")

grid.columnnames <- c(General="General",
                      Glycine="Glycine",
                      Proline="Proline",
                      Pre.Pro="Pre-Pro")

grid.levels <- t(cbind(General=c(0, 0.0005, 0.02, 1),
                       Glycine=c(0, 0.002,  0.02, 1),
                       Proline=c(0, 0.002,  0.02, 1),
                       Pre.Pro=c(0, 0.002,  0.02, 1)))

grid.colors <- t(cbind(General=c('#FFFFFF','#B3E8FF','#7FD9FF'),
                       Glycine=c('#FFFFFF','#FFE8C5','#FFCC7F'),
                       Proline=c('#FFFFFF','#D0FFC5','#7FFF8C'),
                       Pre.Pro=c('#FFFFFF','#B3E8FF','#7FD9FF')))

grid.dir <- "top500-angles/pct/rama/"
scatter.filename <- "1HMP.tsv"
```

The following loads the example datafile, and then draws the four Ramachandran plots, using the specified four distributions loaded from their files:

```
scatter.data <- load.scatter(scatter.filename)

# Split the plot into quadrants:
par(mfrow=c(2,2))

for(rama.type in names(grid.filenames)) {
    # Filter the input data for this graph type
    col.name = grid.columnnames[rama.type]
    scatter.phi <- scatter.data[which(scatter.data[,"type"]==col.name), "phi"]
    scatter.psi <- scatter.data[which(scatter.data[,"type"]==col.name), "psi"]

    # Load the distribution for this graph type
    grid.filename <- paste(grid.dir, grid.filenames[rama.type], sep="")
    grid <- load.grid(grid.filename, mid.points)

    # Use small margins to make the plots nice and big, which as a
    # side effect means squeezing the axes labels a bit, and specify
    # a SQUARE plot area (to go with aspect ratio, asp=1)
    par(mar=c(3,3,3,3), mgp=c(1.75,0.75,0), pty="s")

    ramachandran.plot(scatter.phi, scatter.psi,
             x.grid=mid.points, y.grid=mid.points, z.grid=grid,
             plot.title=col.name,
             levels=grid.levels[rama.type,],
             col=grid.colors[rama.type,])
}
```



Downloads

You might want the following files:

- 1hmp_mmtk.tsv - Example phi/psi angle input file, tab separated variables
- draw_rama.r - Example R script with all the above code
- Expected occupancy files top500-angles/pct/rama/rama500-*.data from one of the following archives:
    - top500-angles.050606.zip (80MB) (newer, 2005-06-06)
    - top500-angles.040823.tgz (69MB) (older, 2004-08-23)
    - Readme file

But I Like Python!

Don't worry - using RPy you can draw these graphs by calling R from python.

The R Project

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