Visualizing Protein Structures Using Plotly

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Am I the first one to try to visualize protein structures using Plotly?

Personally, I think the hitherto most powerful and elegant protein structure visualization tool is SwissPdbViewer (a.k.a. DeepView), which is tightly linked to SWISS-MODEL. Apparently it's used as a web application, but it is not written in JS. It is not open source, and it's 32-bit architecture makes it obsolete on modern 64-bit computers.

Plotly has an open source graphing library with APIs for R, Python and JS, of which the R API highly compatible with the renowned `ggplot2` package. This means you can make ggplots in R and convert them into interactive svg images for web with one line of code!

Apart ggplot conversion, Plotly also provides its own suite of plotting functions in its R API, many of which are specifically suited for web application (e.g. 3D support).

Given its simplicity and rich APIs, I think Plotly might be used as a framwork for plotting protein structures. In this preliminary experiment, I plotted the atoms of a protein structure (written in a PDB file) as dots with Plotly in R, and rendered them into HTML widgets in Rmarkdown, so that the plots shown below are interactive!

Required Packages:

```r
library(tidyverse)
library(plotly)
library(Rpdb)
```

```r
x <- read.pdb('/Users/tianyishi/Desktop/sample.pdb')
pdb <- as_tibble(x$atoms) %>%
  mutate(charge = ifelse(resname %in% c('LYS', 'ARG', 'HIS'),
                         'basic', ifelse(resname %in% c('ASP', 'GLU'),
                                          'acidic', 'neutral')))
```

```r
pdb %>% plot_ly(x = ~x1, y = ~x2, z = ~x3, color = ~charge, colors = c('red', 'blue', 'grey')) %>%
  add_markers()
```

```r
pdb %>% plot_ly(x = ~x1, y = ~x2, z = ~x3, color = ~resname) %>%
  add_markers()
```