Contents


```
% Solution to Assignment 6: Andrew Gerst

clear all; close all;
```

Function Descriptions

readPDBfile Function

This function reads the atoms for a protein and returns their serial number, atom name, and coordinates.

```
type readPDBfile
```

```
function [anum, aname, coords] = readPDBfile(infile)
% This function reads the atoms for a protein and returns their serial
% number, atom name, and coordinates.

        fid = fopen(infile,'rt');
    if fid == -1
        return
    end
    anum = []; aname = []; coords = [];
    while ~feof(fid)
        line = fgetl(fid);
        record = line(1:6);
        num = line(7:11);
        name = line(13:16);
        seqnum = line(23:26);
        xcoord = line(31:38);
        ycoord = line(39:46);
        zcoord = line(47:54);
        coord = [str2double(xcoord) str2double(ycoord) str2double(zcoord)];
        if strcmp(record,'ATOM  ')
            anum = [anum;str2num(num)];
            aname = [aname;upper(name)];
            coords = [coords;coord];
        end
    end
    aname = strtrim(aname);
    fclose(fid);
end
```

potentialHbonds Function

This function looks for any possible pairs of Nitrogen and Oxygen between a distance of 2.6 and 3.2 angstroms. Returns a list containing the pairs of atom numbers for hydrogen bonding pairs.

```
type potentialHbonds
```

```
function pairs = potentialHbonds(anum, aname, coords)
% This function looks for any possible pairs of Nitrogen and Oxygen between
% a distance of 2.6 and 3.2 angstroms. Returns a list containing the pairs
% of atom numbers for hydrogen bonding pairs.

    pairs = [];
    name = cellstr(aname);
    nitrogen = [];
    oxygen = [];
    for idx = 1:length(name)
        if name{idx}(1) == 'N'
            nitrogen = [nitrogen idx];
        elseif name{idx}(1) == 'O'
            oxygen = [oxygen idx];
        end
    end
    for ii = 1:length(nitrogen)
        for jj = 1:length(oxygen)
            n_idx = nitrogen(ii);
            o_idx = oxygen(jj);
            d = sqrt((coords(n_idx,1)-coords(o_idx,1))^2 + (coords(n_idx,2)-coords(o_idx,2))^2 + (coords(n_idx,3)-coords(o_idx,3))^2);
            if d > 2.6 && d < 3.2
                pairs = [pairs; [anum(n_idx) anum(o_idx)]];
```

```
            end
        end
    end
end
```

drawAtoms Function

This function plots any atoms with aname matching the queryName.

```
type drawAtoms
```

```
function ret = drawAtoms(queryName, marker, aname, coords)
% This function plots any atoms with aname matching the queryName.

    query = strtrim(queryName);
    name = cellstr(aname);
    coord = [];
    for idx = 1:length(name)
        if strcmp(query,name{idx})
            coord = [coord; [coords(idx,1) coords(idx,2) coords(idx,3)]];
        end
    end
    plot3(coord(:,1),coord(:,2),coord(:,3),marker);
end
```

Protein 7HVP

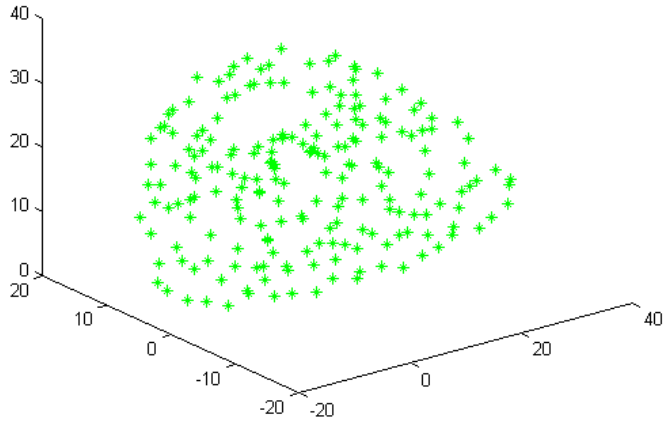
```
[anum aname coords] = readPDBfile('7HVP.pdb');

% Generate 3D Plot of C atoms
drawAtoms(' C  ', 'g*', aname, coords);

% Output number of hydrogen bonds
pairs = potentialHbonds(anum, aname, coords);
numOfHbondPairs = length(pairs)
```

```
numOfHbondPairs =

   286
```



Protein 1GFL

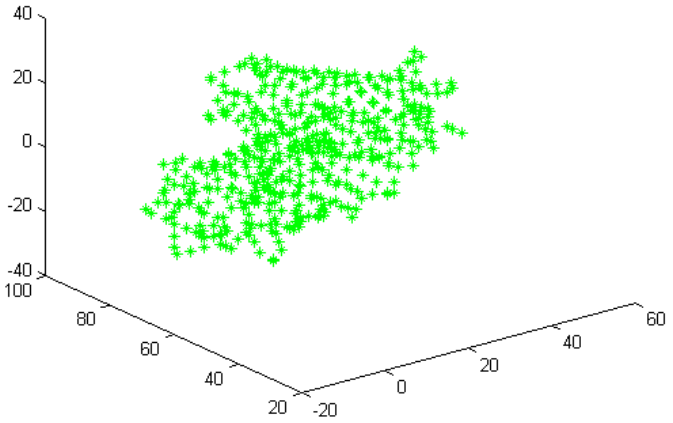
```
[anum aname coords] = readPDBfile('1GFL.pdb');

% Generate 3D Plot of C atoms
drawAtoms(' C  ', 'g*', aname, coords);

% Output number of hydrogen bonds
pairs = potentialHbonds(anum, aname, coords);
numOfHbondPairs = length(pairs)
```

```
numOfHbondPairs =

   775
```



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