MANUAL for: Protein structure quality assessment based on the distance profiles of consecutive backbone $C\alpha$ atoms

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Installation

1. You have to use the tcsh shell (bash shell wont work).

2. You have to install the cpan perl packages from http://www.cpan.org/. The list depends on the program you use, just run the main program - and it will prompt you about the missing packages. Go ahead and install those.

3. You need to set some environment variables (SRC, BIOPERLHOME, etc). The complete list is in a file called "setup.csh" - you need to change this file and source it. This changes the $path variable too.

Running the program

1. $SRC/ALIGN/proquad.pl -outfile out -list list

The file "list" should contain the list of PBDs which needs to be checked. These PDB files are to be kept in a directory, and the variable PDBDIR needs to be set to this directory.

Output

The output gives the CADistScore for each protein. An example for the fisa decoy set.
1FC2 averageCAist1000 = 0.006
AXPROA00-MIN averageCAist1000 = 0.024
AXPROA01-MIN averageCAist1000 = 0.018
AXPROA02-MIN averageCAist1000 = 0.02
AXPROA03-MIN averageCAist1000 = 0.021
AXPROA04-MIN averageCAist1000 = 0.02
AXPROA05-MIN averageCAist1000 = 0.019
AXPROA06-MIN averageCAist1000 = 0.02
AXPROA07-MIN averageCAist1000 = 0.022
AXPROA08-MIN averageCAist1000 = 0.021
AXPROA09-MIN averageCAist1000 = 0.02
AXPROA10-MIN averageCAist1000 = 0.021
AXPROA11-MIN averageCAist1000 = 0.021
AXPROA12-MIN averageCAist1000 = 0.022