This code constructs an HANM on the basis of input protein structure file using the PFM method. The output model can reproduce experimental B-factors and generate normal modes.

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COMPILING
To compile the code, you need GNU Scientific Libary (GSL) installed in your path. Please refer to http://www.gnu.org/software/gsl/ for details. Then compile and link the code using:
gcc HANM.c -o HANM -lgsl -lgslcblas -lm -O3

RUNNING
>> Usage: HANM ca.pdb k0 cutoff factor mcycles ncycles (fcfile)!

The parameters are:
ca.pdb --> PDB file containing coordinates of Ca atoms.
k0 --> Start with this uniform force constant, leave it 0 to use the optimal force constant of ANM.
cutoff --> Atom pairs of distances within the cutoff will be connected by a harmonic spring.
factor --> How large a restraint potential will be added in each cycle. The restraint force constant is factor*KBT*8pi^2*(Bcal-Bexp)/(Bcal*Bexp).
mcycles --> Number of outer cycles to update B factors.
ncycles --> Number of Inner cycles for fluctuation matching.
Fcfile --> (Optional) Read the initial force constants from this file. The file fcfile contains lines as "atomA atomB fcAB". For example, "1 2 1000" means to connect atom 1 and atom 2 by a harmonic spring with the force constant 1000 kJ/mol/nm^2.

OUTPUT
The output includes the calculated B-factors and spring constants.

Please refer to the source code for more details.