A

Single PDB | Comparative

PDB ID 4ake

PDB structure file Browse... No file selected.

Chains

E-Mail

Start default analyses ?

Run analysis

max. 20 000 amino acids

Set example input

B

Webnma

apps.cbu.uib.no/webnma/jobs/2014-07-04-11-58-29-964294

WEBnm@

Webtool for Normal Mode Analysis

Version 2.0

Home Howto Web-services About Contact

Performing pre-analysis computations

Please wait...

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C

Warnings

* 4ake.pdb:
Only alpha-carbon records of standard amino acids are used in the model for normal mode analysis. Other records are ignored.

Input

Your input for this analysis was:
4ake

Normal Modes

The lower energy normal modes were calculated and can be downloaded as a whitespace delimited text file: modes.dat . For larger structures, higher modes are not calculated unless needed for numerical convergence.

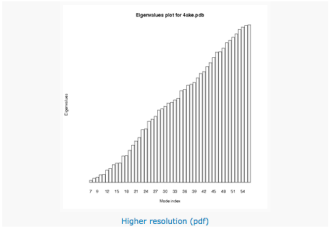
Deformation Energies

Below are the values of the deformation energy for the lowest-frequency non-trivial modes (modes 7 to 20). See more...

| Mode Index | Deformation Energy | Mode Index | Deformation Energy |
|---|---|---|---|
| 7 | 135.96 | 14 | 1350.43 |
| 8 | 211.76 | 15 | 1125.02 |
| 9 | 216.34 | 16 | 1315.82 |
| 10 | 378.89 | 17 | 2048.80 |
| 11 | 435.77 | 18 | 2120.09 |
| 12 | 804.01 | 19 | 2430.89 |
| 13 | 931.19 | 20 | 3163.11 |

Eigenvalues

The eigenvalues for the lowest-frequency non-trivial modes.



Higher resolution (pdf)

Proceed to Analyses

Analyses

Atomic Displacement Analysis

Plots the displacement of each Calpha atom, i.e. highlights which parts of the protein are the most displaced for each mode, and plots the atomic fluctuations of the protein.

Mode Visualization and Vector Field Analysis

Animates the modes in your browser.

It also shows a vector field representation of the modes, i.e vectors are used to show the directions and (relative) amplitude of the displacements undergone by different parts of the protein.

You can also download a DCD trajectory file showing the animation, and a VMD file containing the vector field representation.

Overlap Analysis

Compare the normal modes of your structure with the transition to a different conformation of the same protein. This calculation allows identification of a few modes that can be used to describe the transconformations between the two structures.

The structure provided for the overlap analysis must have the same number of CA-atoms as the one the normal modes were calculated for, and the atoms of the two structures should correspond to each other in the order they appear in the PDB-files. Otherwise strict sequence identity is not enforced.

PDB ID to overlap

PDB file to overlap Browse... No file selected.

Chains

Run analysis

Correlation Matrix Analysis

Plots the correlation between motions of all the Calphas in the protein structure.

Run analysis

Results

Deformation Energies

Download All

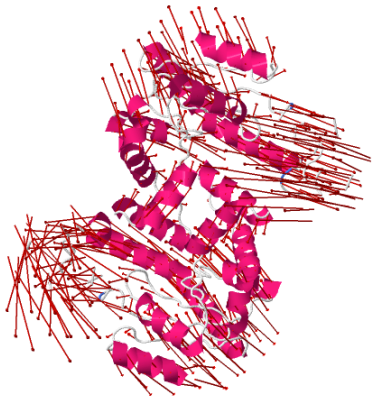
Input

Your input for this analysis was:
4ake

D

Mode Visualization

Shows a vector field representation of the modes. Vectors are used to show the directions and (relative) amplitude of the displacements undergone by different parts of the protein. See more...



Jmol_S

Vibrations Vectors

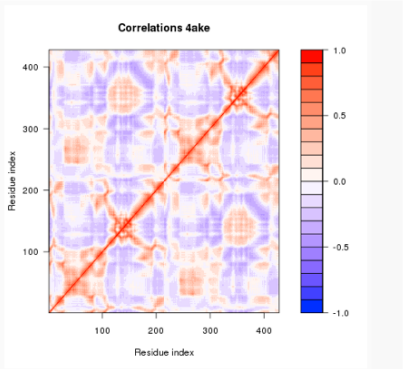
Take a snapshot mode 7

File Download

| Mode 7 | Mode 8 | Mode 9 | Mode 10 | Mode 11 | Mode 12 |
|---|---|---|---|---|---|
| DCD file | DCD file | DCD file | DCD file | DCD file | DCD file |
| VMD file | VMD file | VMD file | VMD file | VMD file | VMD file |

Correlation Matrix Result

The correlation matrix shows the correlated movement of the Calphas in the protein. See more...

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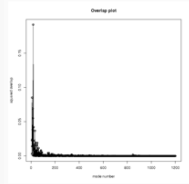
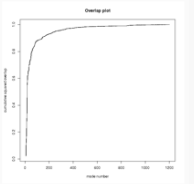
Overlap between normal modes and difference vector

The squared inner product between the difference vector and each of the calculated normal modes identifies which modes contribute most to the structural difference. See more...

The squared inner product (overlap) between the difference vector between the two conformations of the protein and the full set of normal modes.

| Overlap | Cumulative overlap |
|---|---|
|  |  |
| Click to enlarge | Click to enlarge |
| Download DAT file | Download DAT file |
| Download PDF | Download PDF |

Linear Interpolation between the two conformations:

This illustration is not a function of the normal modes, but is provided as an illustration of the conformational change.

Jmol_S