

**A**

**Single PDB** **Comparative**

PDB ID:

PDB structure file:  No file selected.

Chains:

E-Mail:

Start default analyses [?](#)

max. 20 000 amino acids

**B**

Webnma

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

**WEBnm@**  
Webtool for Normal Mode Analysis  
Version 2.0

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Performing pre-analysis computations

Please wait...

**Input**  
Your input for this analysis was:  
4ake

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**C**

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

**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 \(pdf\)](#)

**D**

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**Analyses**

**Atomic Displacement Analysis**  
Plots the displacement of each Alpha 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:  No file selected.

Chains:

**Correlation Matrix Analysis**  
Plots the correlation between motions of all the Calphas in the protein structure.

**E**

**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...](#)

**Input**  
Your input for this analysis was:  
4ake

Vibrations  Vectors  
Take a snapshot:

**File Download**

Mode 7	Mode 8	Mode 9	Mode 10	Mode 11	Mode 12
<a href="#">DCD file</a>	<a href="#">DCD file</a>	<a href="#">DCD file</a>	<a href="#">DCD file</a>	<a href="#">DCD file</a>	<a href="#">DCD file</a>
<a href="#">VMD file</a>	<a href="#">VMD file</a>	<a href="#">VMD file</a>	<a href="#">VMD file</a>	<a href="#">VMD file</a>	<a href="#">VMD file</a>

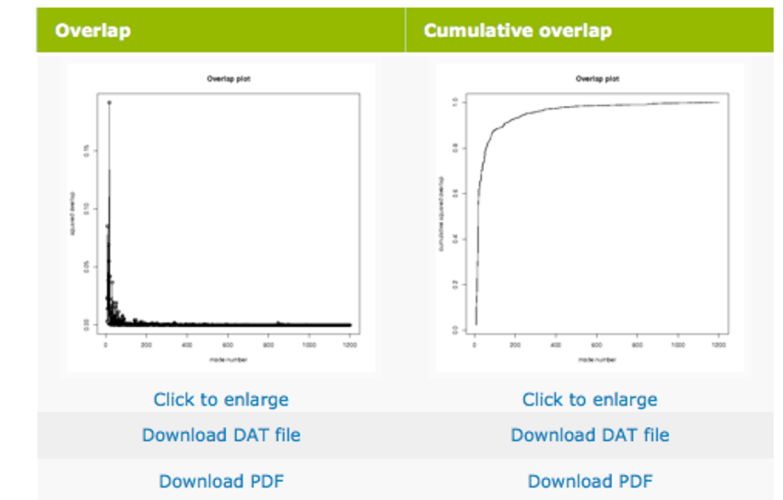
**Correlation Matrix Result**  
The correlation matrix shows the correlated movement of the Calphas in the protein. [See more...](#)

[Higher resolution \(pdf\)](#)  
[Download DAT file](#)  
[Download pymol script](#)

**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.

**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