



Molecular Dynamics on Web

Tutorial, v1.0

Table of Contents

MDWeb Setup Tutorial.....	3
1.- Registration.....	3
2.- Starting Project	4
3.- Checking the Structure	5
4.- Structure Setup.....	7
5.- Waiting Results	9
6.- Getting Results	11
MDWeb Running Simulation Tutorial.....	12
1.- Generating Needed Files	12
2.- Downloading and Extracting Files	13
3.- Preparing Downloaded Files	15
4.- Launching Molecular Dynamics Simulations	17
MDWeb Protein Analysis Tutorial	18
1.- Registration.....	18
2.- Starting Project	19
3.- Uploading a Trajectory	20
4.- Running Analysis.....	22

MDWeb Setup Tutorial

MDWeb provides a friendly environment to setup new systems and run test simulations. With this short tutorial, you will be able to prepare a molecule to run a molecular dynamics simulation, following just a few steps.

1. [Registration](#)
2. [Starting Project](#)
3. [Checking the Structure](#)
4. [Structure Setup](#)
5. [Waiting Results](#)
6. [Getting Results](#)

Tutorial Steps

1. **Registration**

The first thing to do is choose between working as an *anonymous* user or alternatively as a *registered* user. We **strongly** recommend working as a registered user, as it has some important advantages.

Anonymous user's projects are completely removed once the user is disconnected and also when session expires (after some minutes of inactivity), and therefore working as anonymous user is only suited for a first impression of the web server.

[Registration process](#) will just take a minute --> [Registration](#).

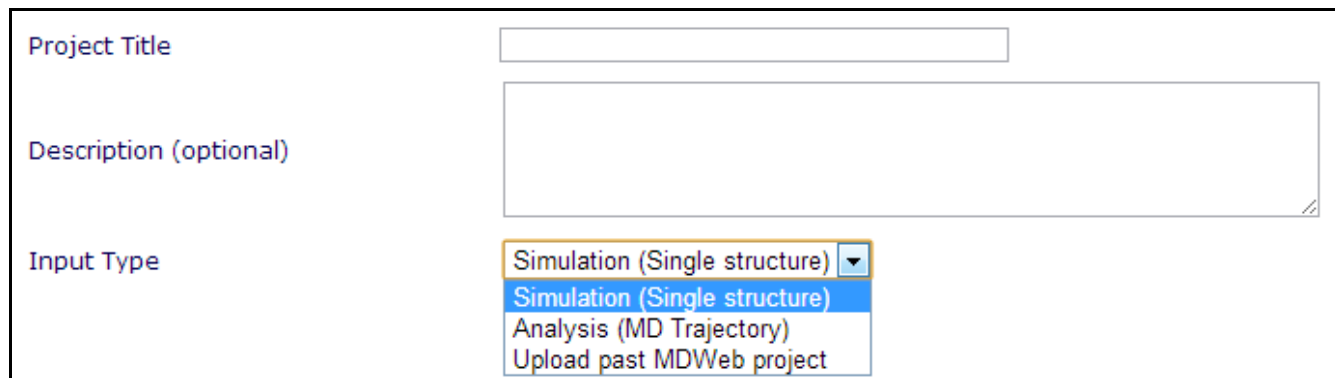
Once logged in, the user **workspace** appears. In this **workspace**, all projects of the user will be shown.

Now, we are ready to start our first **MDWeb** project.



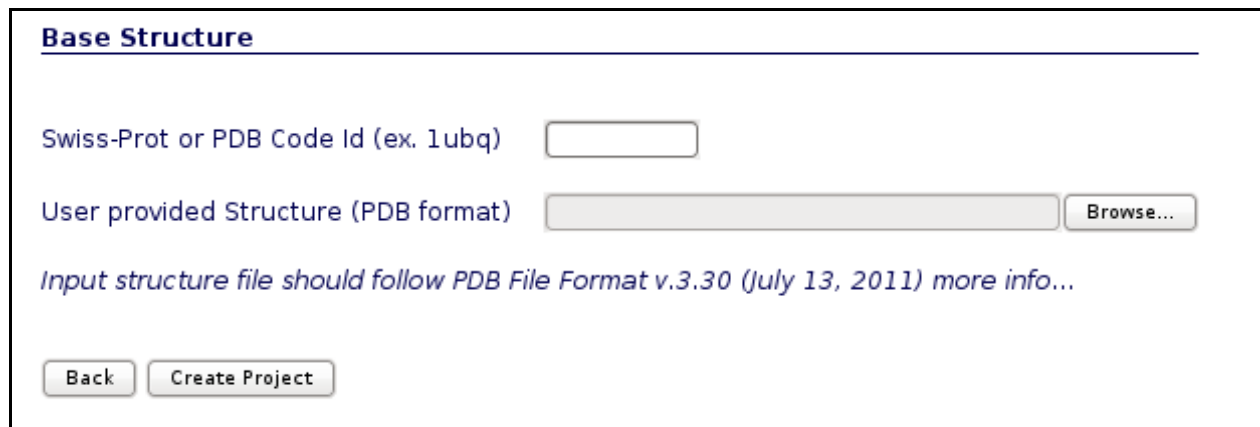
2. Starting Project

MDWeb user can choose between four different kind of inputs, *Simulation*, *Analysis*, and *Upload a past MDWeb project*. In this tutorial, we will see an example of a Setup (Simulation) project.



The screenshot shows a web form for creating a project. It has three main sections: 'Project Title' with a text input field, 'Description (optional)' with a larger text area, and 'Input Type' with a dropdown menu. The dropdown menu is open, showing four options: 'Simulation (Single structure)' (highlighted in blue), 'Simulation (Single structure)', 'Analysis (MD Trajectory)', and 'Upload past MDWeb project'.

You will be asked for just three easy inputs: a project title, an optional description of the project, and an input structure, either as a **PDB code** or directly as a **PDB structure file**.



The screenshot shows the 'Base Structure' section of the form. It has a title 'Base Structure' followed by a horizontal line. Below the line are three input fields: 'Swiss-Prot or PDB Code Id (ex. 1ubq)' with a text input field, 'User provided Structure (PDB format)' with a text input field and a 'Browse...' button, and a note: 'Input structure file should follow PDB File Format v.3.30 (July 13, 2011) more info...'. At the bottom are two buttons: 'Back' and 'Create Project'.

3. Checking the Structure

Just after creating the project, you will be redirected to the so-called *Checking page*. In this page, **MDWeb** will show a list of possible problems found in the input structure that can affect to a future Molecular Dynamics Simulation. User can interactively inspect these problems thanks to a Jmol applet coupled to each of the problems, helping to locate them on the real tridimensional structure.

In this particular case, we are trying to work with the well-known *Ubiquitin chromosomal protein* (pdb code 1ubq). At the right part of the screen, you will find all the possible problems identified, whereas at the left part of the screen the Jmol applet with the structure loaded will be shown.

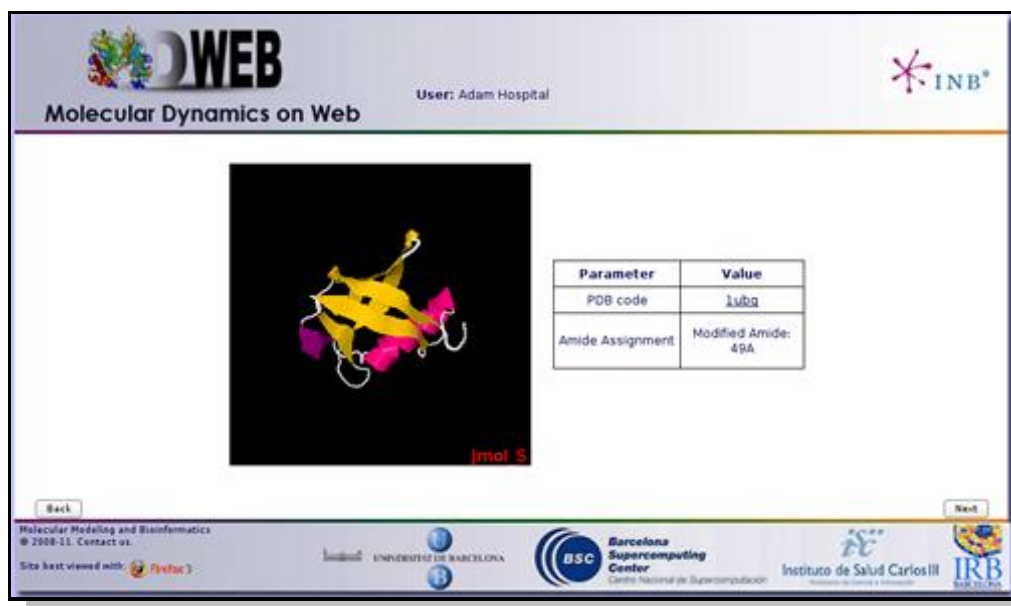
This small protein, with less than 80 aminoacids, has just two possible problems, marked as a warning symbol ⚠ or as an error symbol ✖ in the problem list.

Warning messages are identified problems that can sometimes be adjusted/corrected in this same page. For example in this case there is an **amide incorrect assignment** in the residue number 49, that can be fixed with just a click in the desired button. The identification of this type of problems (together with all the possible problems checked) is described in the correspondent help section ([Structure Checking](#)).

Error messages are identified problems that will probably cause Molecular Dynamics failure. The typical example is the one found in our example protein, an *atom clash*. Our ubiquitin protein has a pair of **Polar Acceptor atoms** too close (two oxygen atoms specifically, as you can perfectly see in the JMol applet), just 3Å away. In this case, a simple energetic minimization of the system will put these pair of oxygen appart from each other, but sometimes a clash like this can be extremely dangerous for a Molecular Dynamics Simulation. **Atomic clashes** and **Sequence Gaps** are two of the most relevant problems in running MD simulations. More information about them can be found in the correspondent help section ([Structure Checking](#)).

Note that in this example, a **Polar Donor Clash** appears when we first load the structure, but it disappears when user fixes the **incorrect amide assignment** and the clashes are recomputed.

When clicking the next button, an **intermediate information page** will appear, listing the most important information chosen in the previous *Checking* page, i.e. **amide assignments** and **ligands discarded/taken**, and showing the part of the structure (chain/s) chosen for the project in a JMol applet.




The screenshot displays the MDWeb interface. At the top left is the MDWEB logo, and at the top right is the INB logo. The user is identified as Adam Hospital. The main content area features a JMol applet showing a protein structure with yellow and pink components. To the right of the applet is a table with the following data:

Parameter	Value
PDB code	1ubq
Amide Assignment	Modified Amide: 49A

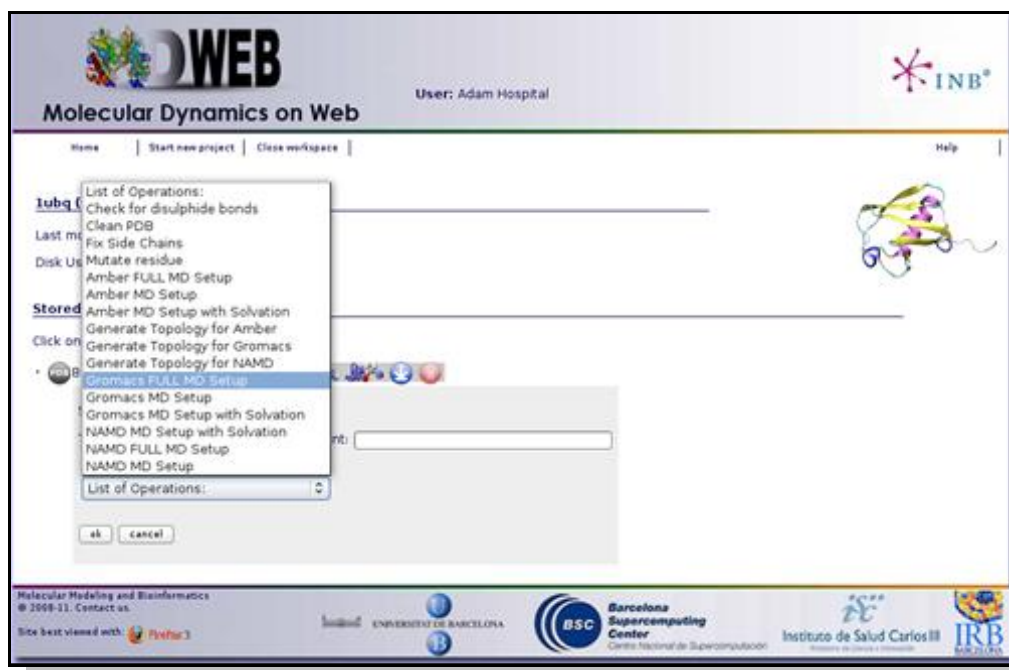
At the bottom of the interface, there are navigation buttons for 'Back' and 'Next', and a footer containing logos for Molecular Modeling and Bioinformatics, Universitat de Barcelona, BSC (Barcelona Supercomputing Center), Instituto de Salud Carlos III, and IRB.

In this particular case, we just did a modification in one amide, on the residue 49.

4. Structure Setup

At this point, we already have our structure loaded into **MDWeb** workspace. Now we are going to choose a **workflow** from the list of possible operations, after clicking at the *New Operation* icon . Our goal is obtain a system completely prepared to begin a Molecular Dynamic Simulation with **Gromacs** package. So we will click at the operation named: **Gromacs FULL MD Setup**. Note that choosing operation **Namd FULL MD Setup**, a system for **Namd** Package with **Charmm** forcefield will be prepared, and choosing **Amber FULL MD Setup**, a system for **Amber** Package with **Amber** forcefields will be prepared.

Gromacs FULL MD Setup will run a complete **Molecular Dynamics Setup** to the input structure. That means going from a protein/nucleic acid structure to a system formed by the molecule submerged into a solvent box, surrounded by ions up to a given concentration, and energetically equilibrated. For a more extended information about the steps done by the workflow, see the corresponding help section ([Gromacs Workflow FULL Setup](#)).



After clicking at the workflow **Gromacs FULL MD Setup**, it will give us the possibility to choose between a set of different **forcefields**. A force field has three components: equations defining the potential energy of a molecular system as a function of atomic coordinates, atom types, and parameter sets that fit the equations to experimental data. We will just keep the option that is active by default in **MDWeb**. In this case, **Amber-99SB*** forcefield.

MDWEB
Molecular Dynamics on Web

User: Adam Hospital

Home | Start new project | Close workspace | Help

1ubq (MDWebdf227d8d52d0a)

Last modification on: 27/01/2012 11:33
Disk Usage: 1.2 MB

Stored structures

Click on structure title to deploy the toolbox.

Base structure (78.1 kB)

Select the desired operation.

Title: Comment:

Gromacs FULL MD Setup

Forcefield: AMBER-99SB* force field


- GROMOS96 43a1 force field
- GROMOS96 43a2 force field (improved alkane dihedrals)
- GROMOS96 45a3 force field (Schuler JCC 2001 22 1205)
- GROMOS96 53a5 force field (JCC 2004 vol 25 pag 1656)
- GROMOS96 53a6 force field (JCC 2004 vol 25 pag 1656)
- OPLS-AA/L all-atom force field (2001 aminoacid dihedrals)
- [DEPRECATED] Gromacs force field (see manual)
- [DEPRECATED] Gromacs force field with hydrogens for NMR
- Encad all-atom force field, using scaled-down vacuum charges
- Encad all-atom force field, using full solvent charges
- AMBER-94 force field
- AMBER-96 force field
- AMBER-99 force field
- AMBER-03 force field (all-atom only, does not include the AMBER-03ua united-atom potential)
- AMBER-GS force field
- AMBER-GS-S force field (no 1-4 vdW scaling)
- AMBER-99f force field
- AMBER-99SB force field
- AMBER-BSC0 force field
- AMBER-99SB* force field

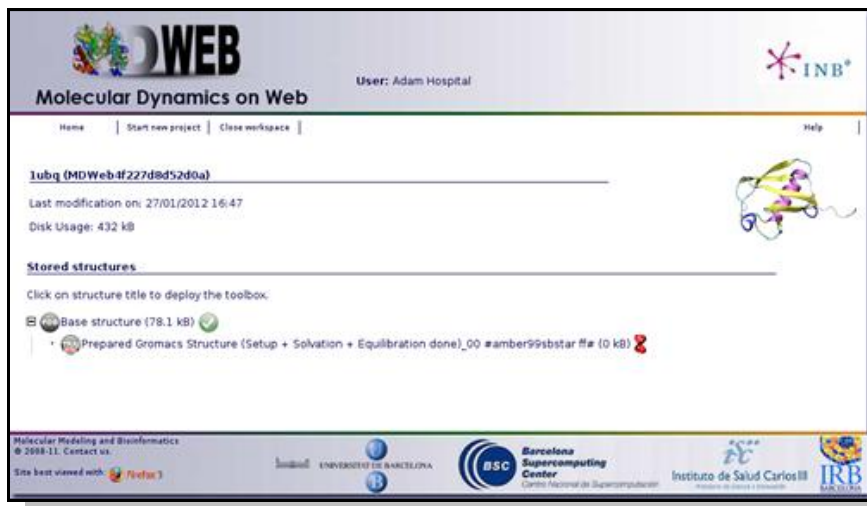
Molecular Modeling and Bioinformatics
© 2008-11. Contact us


Site best viewed with:

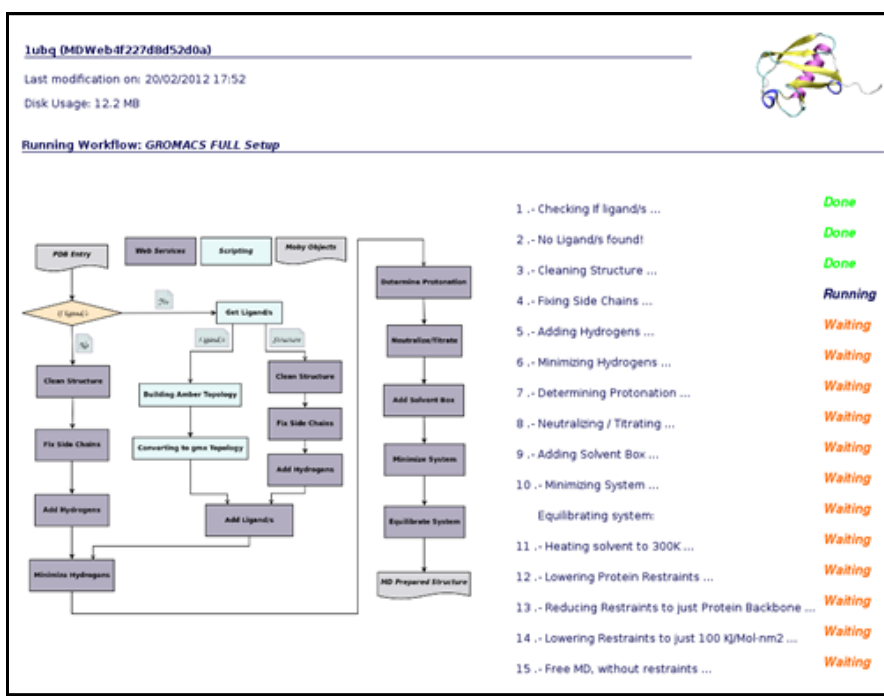
Instituto de Saú Carlos III
IRB
MADRID

5. Waiting Results

Once the workflow is launched, we just have to wait for the results. **MDWeb** will be automatically reloaded from time to time after checking if the process has already finished. Meanwhile, you can follow the progress of it clicking at the sandclock  whenever you want.



When clicking at the **sandclock** , a new page will be opened showing the progress of the workflow step by step, accompanied by a figure of the whole workflow. This way, you will be able to know at any moment which service is being executed, how many steps have been already computed, and how many steps left.



MDWeb offers you the possibility to leave your processes running (as sometimes they will be long processes), disconnect from the server, and reconnect again later on, to check the progress of your projects. The list of projects is easily accessible from the user workspace page.




The screenshot displays the MDWeb user workspace interface. At the top, the MDWeb logo is on the left, the user name "User: Adam Hospital" is in the center, and the INB logo is on the right. Below the header, there are navigation links: "Home", "Start new project", "Class workspace", "Analysis Tutorial", "Setup Tutorial", and "Help".

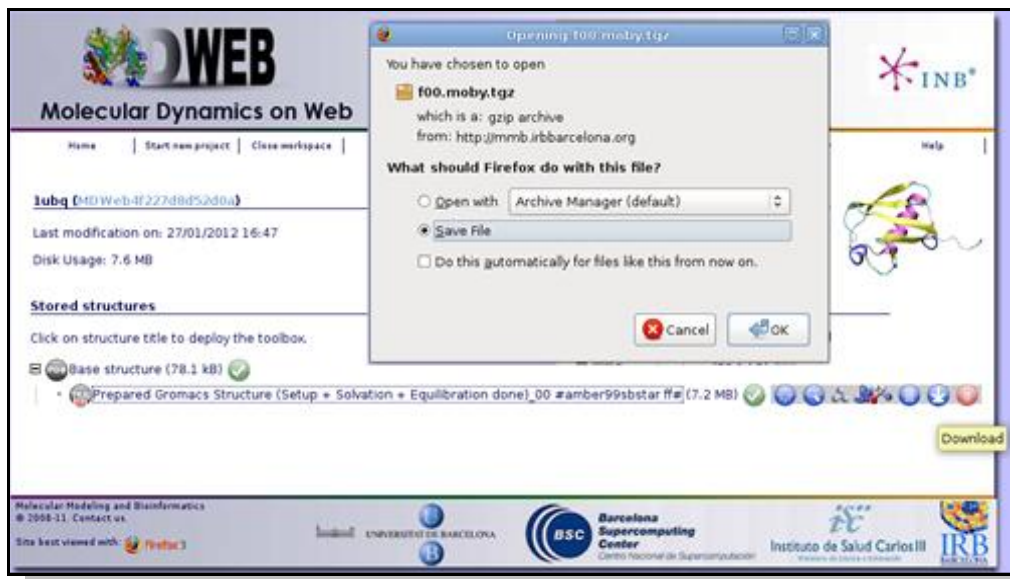
The main section is titled "Stored projects" and shows a "Total Disk Usage: 669.7 MB". Below this, a list of projects is displayed, each with a status icon (a blue circle with a white smiley face) and a red circle with a white 'X' icon. The projects listed are:

- 4ake. Last Modified on 09/02/2012 12:05 (13.9 MB);
- 1ake. Last Modified on 26/01/2012 17:28 (6.7 MB);
- MDWeb Tutorial: 1ubq. Last Modified on 20/02/2012 13:32 (127.8 MB);
- 1ubq. Last Modified on 02/02/2012 16:50 (19.2 MB);
- 1agj. Last Modified on 02/02/2012 18:25 (91.6 MB);
- 2k5. Last Modified on 27/01/2012 19:26 (4.7 MB);
- 1k5. Last Modified on 01/02/2012 17:42 (1.6 MB);
- 2k5_lq. Last Modified on 02/02/2012 13:51 (116.9 MB);
- 1fd. Last Modified on 09/02/2012 12:18 (5.9 MB);
- 2k5. Last Modified on 10/02/2012 11:11 (6.4 MB);
- 1kqw. Last Modified on 10/02/2012 13:56 (14.4 MB);
- Senne Hydrolase MD Analysis. Last Modified on 10/02/2012 18:16 (120 MB);

The footer contains copyright information: "Molecular Modeling and Bioinformatics © 2008-11. Contact us." and logos for "INB", "UNIVERSITAT DE BARCELONA", "RSC Barcelona Supercomputing Center", "Instituto de Salud Carlos III", and "IRB".

6. Getting Results

Once the workflow has finished, you have the possibility to download the data generated, just clicking at the *download* icon .



Now you can work with your system, already prepared to run an MD Simulation with **Gromacs** package. The downloaded compressed file has all the necessary inputs to run the simulation, but still you will need to prepare the configuration file needed by gromacs to begin the run with some key parameters like the **MD ensemble, simulation time, time step**, etc. But don't worry, if you are not familiar at all with **Gromacs**, MDWeb will help you preparing these configuration input files for you. Check [Run Simulation Tutorial](#).

This example is done with Gromacs package, but MDWeb also offers a complete setup workflow for working with Namd package with **Charmm** forcefield or **Amber** forcefields. The complete list of workflows can be found at help pages ([MDWeb List of Workflows](#)).

MDWeb Running Simulation Tutorial


MDWeb provides a friendly environment to setup new systems and run test simulations. With this short tutorial, you will be able to run a **Molecular Dynamics Simulation** in your own machines, using files provided by **MDWeb** after preparing the system.

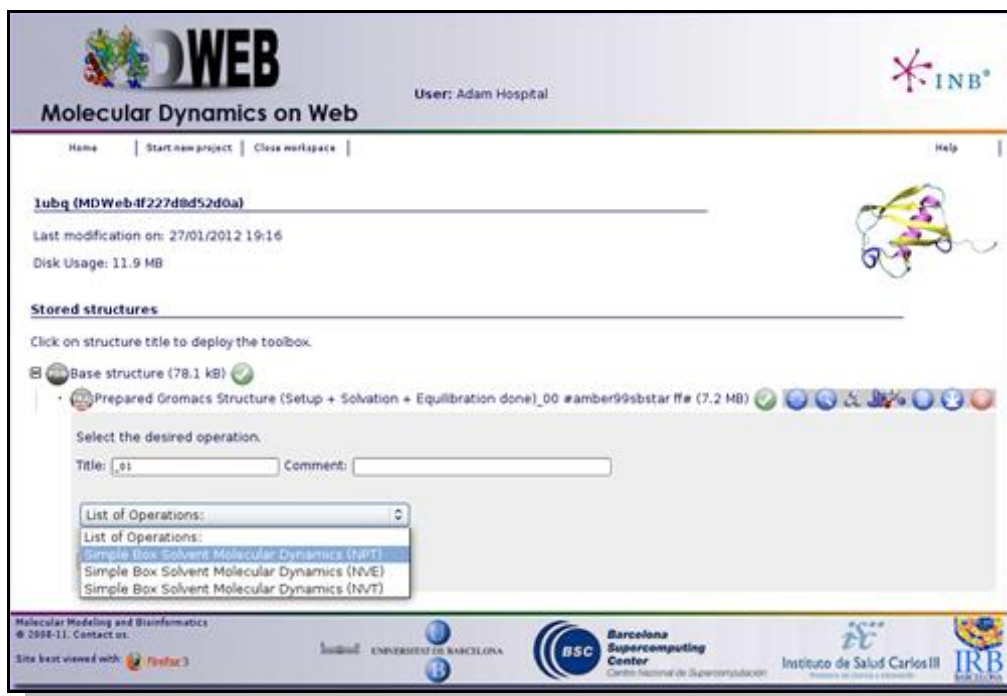
1. [Generating needed files](#)
2. [Downloading and Extracting Files](#)
3. [Preparing Downloaded Files](#)
4. [Launching Molecular Dynamics Simulation](#)

Tutorial Steps

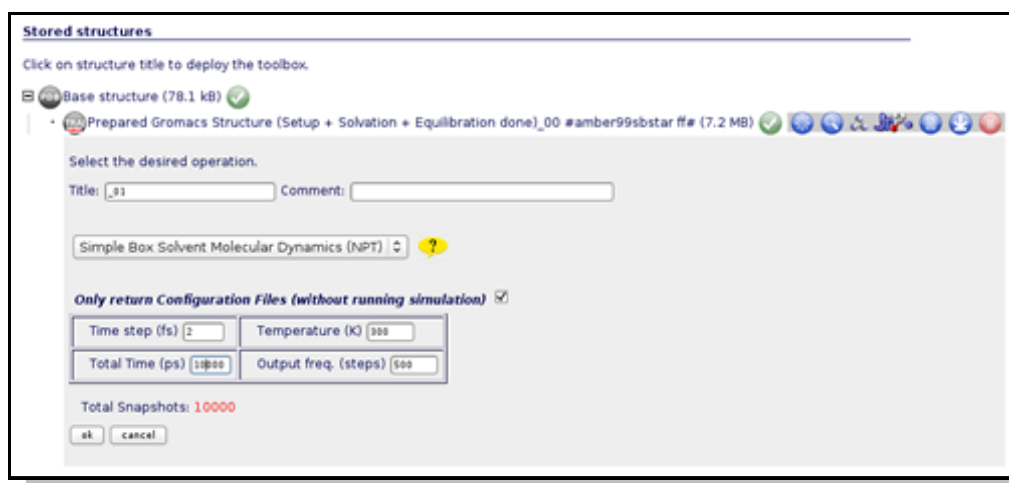
1. Generating needed files

This short tutorial assumes that user have already setup a system using one of **MDWeb** Workflows to run a complete system preparation: *GromacsWorkflowFULL*, *AmberWorkflowFULL*, or *NamdWorkflowFULL* (see [Setup Tutorial](#)), or alternatively it has been prepared step by step using the appropriate **MDWeb** operations.

The first thing to do then is run an operation called *Simple Box Solvent Molecular Dynamics* with the MD ensemble of interest (**NPT**, **NVE** or **NVT**). It can be found in the **MDWeb Simulation Operations**, clicking at the icon .




We will need to fill in the parameter fields with desired values. For example, if what we want is to run a **Molecular Dynamics Simulation** of 10 ns with a timestep of 2 fs at a 300 K of temperature (a standard molecular dynamics first step, to completely equilibrate the system), we just have to write these numbers: **Time Step: 2 fs**, **Temperature: 300 K**, **Total Time: 10000 ps**, and **Output Frequency: 500 steps**. Note that for choosing the output frequency, the total number of snapshots that will be written by the MD Simulation are computed on the fly and shown in red color. In this case, we have chosen to write every 500 steps in order to have 10000 snapshots, one per picosecond.



Note the line saying: **Only return Configuration Files (without running simulation)**. Leaving this checked **MDWeb** will give you all the necessary input files to run the simulation, together with a README file with instructions about how to run it. Unchecking this line, **MDWeb** will perform the simulation, however, in the present case you will get an error message, because only simulations up to 5 ps are allowed in our server due to the limitations in computer resources.

2. Downloading and Extracting Files

Now, in the last operation results, we have to click at the download icon  to get all the necessary files to run the **prepared Simulation**. The file downloaded is a gzip-compressed tar file, which can be easily uncompressed and unpacked with the appropriate program.

The list of files extracted, depending on the Workflow Program, looks like this:

[GROMACS Files:](#)

<u>File Extension</u>	<u>File information</u>
pdb	MD Input coordinate file in PDB format.
gro	MD Input coordinate file in GRO format.
top	MD Input structure topology.
itp	MD Input include topology files.
ndx	MD Input index file, containing user definable sets of atoms.
trr	MD Input restart file, storing periodic box information, velocities and positions of all atoms.
edr	MD Input restart energy file, storing energies, temperature, pressure, box size, density and virials.
mdp	GROMACS Input configuration file.
gromacs	README.gromacs , explaining how to run the simulation.
tpr	MD Run Input File, in binary format, containing the starting structure of your simulation (coordinates and velocities), the molecular topology and all the simulation parameters.
	queueSP* --> C-shell script to run MD simulation on a single processor.
	queueMPI* --> C-shell script to run MD simulation on multiple processors with MPI.
sh	queueSGE* --> C-shell script to run MD simulation on a queue manager (SGE).

[NAMD Files:](#)

<u>File Extension</u>	<u>File information</u>
pdb	MD Input coordinate file in PDB format.
psf	MD Input structure topology.
xsc	MD Input eXtended System Configuration.
pos	MD Input structure positions.
vel	MD Input structure velocities.
in	NAMD Input configuration file.
namd	README.namd file, explaining how to run the simulation.
	queueSP* --> C-shell script to run MD simulation on a single processor.
	queueMPI* --> C-shell script to run MD simulation on multiple processors with MPI.
sh	queueSGE* --> C-shell script to run MD simulation on a queue manager (SGE).

AMBER Files:

<u>File Extension</u>	<u>File information</u>
pdb	MD Input coordinate file in PDB format.
top	MD Input structure topology (PRMtop format).
in	AMBER Input configuration file.
amber	README.amber file, explaining how to run the simulation.
	queueSP* --> C-shell script to run MD simulation on a single processor.
sh	queueMPI* --> C-shell script to run MD simulation on multiple processors with MPI.

A **README** file for each of the programs explains briefly how to use the given **scripts** to run the simulation. Let's take a look at one example. We will use the preparation done in the [Setup Tutorial](#) help part, with a **GROMACS Workflow**.

3. Preparing Downloaded Files

First of all, let's take a look at the **README** file. In one section, it is said that a few lines of the shell scripts **queue*** need to be modified before launching the simulation. They refer to MD program paths and libraries. These are enclosed between these marks:

```
#####
#
# Modify the following lines according to your installation
#
--> Lines to modify <--
#####
```

So we are going to edit the file named **queueSP***, that corresponds to a **single processor** run. The same should be done with the corresponding **queueMPI*** file to launch the simulation in **Multiple Processors** or with **queueSGE*** to use SGE queue manager.

```
#####
#
# Modify the following lines according to your installation
#
# Path to GROMACS
set GROMACS=/usr
# GROMACS mdrun binary, uncomment as necessary
set MDRUN=$GROMACS/bin/mdrun
#set MDRUN=$GROMACS/bin/mdrun_mpi
#set MDRUN=$GROMACS/bin/mdrun_d

# GROMACS trajconv executable, uncomment as necessary
set TCONV=$GROMACS/bin/trjconv
#set TCONV=$GROMACS/bin/trjconv_d

#####
```

In our case, we know that our Gromacs mdrun executable is located at **/opt/gromacs/bin/**, so we just need to modify the *Path to GROMACS* variable.:

```
set GROMACS=/usr
```

to this new one:

```
set GROMACS=/opt/gromacs
```

The **trjconv** binary is located at the same directory, so we don't have to modify the line:

```
set TCONV=$GROMACS/bin/trjconv
```

And that's all! We already have our shell script prepared to launch the simulation.

4. Launching Molecular Dynamics Simulation

Once again, a section of the README file can help us in this task. It is said that if executing in Single Processor mode, we just need to type:

ssh queueSP* & *where queueSP* can be replaced by the complete real name of the csh file.*

And if all was fine, you will be able to follow the progress of your simulation from the output file named *_**mdrun.log**, where information about the completed and remaining steps is written, together with an estimation of the finishing time:

```
starting mdrun 'Protein in water'
5000000 steps, 10000.0 ps.
step 0

NOTE: Turning on dynamic load balancing

vol 0.80 imb F 2% step 100, will finish Tue Oct 18 11:20:51 2011
vol 0.81 imb F 1% step 200, will finish Tue Oct 18 11:49:35 2011
vol 0.80 imb F 1% step 300, will finish Tue Oct 18 07:22:22 2011
vol 0.80 imb F 0% step 400, will finish Tue Oct 18 05:08:26 2011
...
```

For launching simulations with other packages (**AMBER** and **NAMD**), the steps of this short tutorial should be completely equivalent.

MDWeb Protein Analysis Tutorial

MDWeb provides a friendly environment to analyse your own generated molecular dynamics trajectories. With this short tutorial, you will be able to upload a trajectory and run a set of analysis, checking for example the stability of your system or information about flexibility.

1. [Registration](#)
2. [Starting Project](#)
3. [Uploading a trajectory](#)
4. [Running Analysis](#)

Tutorial Steps

1. Registration

The first thing to do is to choose between working as an *anonymous* user or alternatively as a *registered* user. We **strongly** recommend working as a registered user, as it has some important advantages.

Anonymous user's projects are completely removed once the user is disconnected and also when session expires (after some minutes of inactivity), and therefore working as anonymous user is only suited for a first impression of the web server.

[Registration process](#) will just take a minute --> [Registration](#).

Once logged in, the user **workspace** appears. In this **workspace**, all projects of the user will be shown.

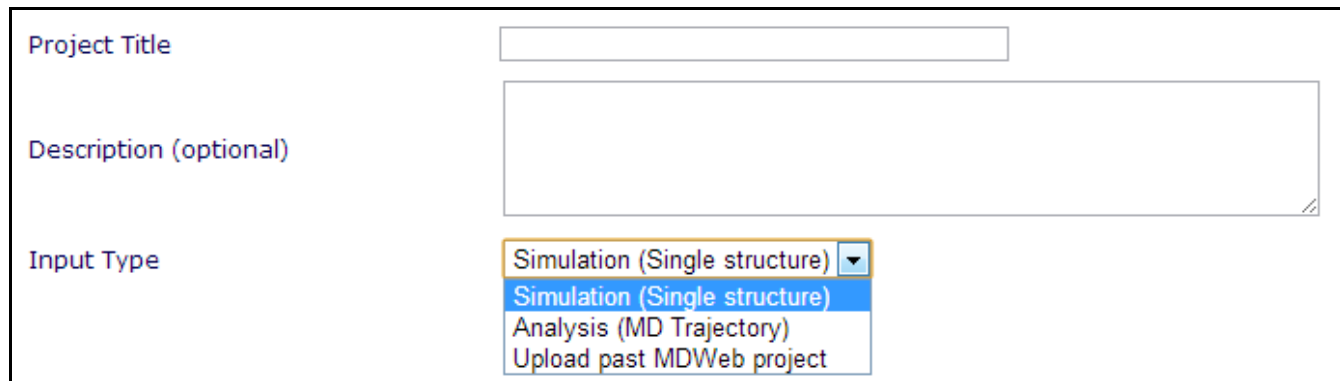
Now, we are ready to start our first **MDWeb** analysis project.



2. Starting Project

MDWeb user can choose between two different kinds of inputs, *Simulation* and *Analysis*. In this tutorial, we will see an example of an *Analysis* project.

You will be asked for a small set of data and input files: First of all, you may fill in a project title and a description (optional) at the top part of the form. Then, at the *Input Type* drop-down selector, just under the description, you should choose the option *Analysis (MD Trajectory)*.



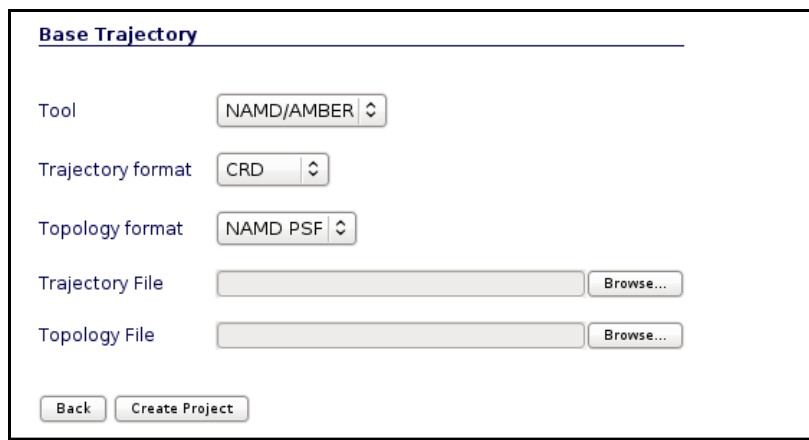
Project Title

Description (optional)

Input Type Simulation (Single structure) ▾

- Simulation (Single structure)
- Simulation (Single structure)
- Analysis (MD Trajectory)
- Upload past MDWeb project

When choosing *Analysis* as input type, a new screen (the one corresponding to *Analysis*, -*MD Trajectory*-) will appear.



Base Trajectory

Tool NAMD/AMBER ▾

Trajectory format CRD ▾

Topology format NAMD PSF ▾

Trajectory File Browse...

Topology File Browse...

Back Create Project

User may select the appropriate **tool, trajectory and topology** format to work with the input files. In the next section we will see an example of how to build the trajectory and topology files with a size small enough to be transferred through the net to **MDWeb** server.

3. Uploading a trajectory

In this example, we are going to compute a set of basic analyses to a 10 ns molecular dynamics simulation of a *Serine Hydrolase* (*pdb code: 1eve*). First of all we need to reduce the size of the **10 ns** trajectory to be uploaded to **MDWeb**. In this case, we will just extract **20 snapshots** from the original obtained trajectory (*one snapshot every 0.5ns*). Alternatively, if you wish to have more resolution, you can extract more snapshots by removing solvent molecules, thus drastically reducing the trajectory file size, but to be able to properly analyse this solvent-stripped trajectory, a coherent topology must be generated, and that's usually not an easy job.

Example of reducing trajectory size:

XTC Trajectory:

Use *trjconv* from [Gromacs](#) package to reduce the size of a trajectory in **XTC** format.

Usage: *trjconv_sp -s structure.gro -f trajectory.xtc -o trajectory.20.xtc -b 1 -e 10000 -dt 500 -ur compact -pbc atom*

where **structure.gro** is the structure topology in **GRO** format, **trajectory.xtc** is the trajectory in **XTC** format, **1-10000** are the starting and ending snapshot times (in ps), and **500** is the offset (write every 500 ps). The rest of the commands are useful when dealing with non-cubic boxes (*-ur*) and periodic boundary conditions (*-pbc*).

You will be asked for a group to write to the output file, e.g.:

Will write xtc: Compressed trajectory (portable xdr format)

Select group for output

Opening library file /usr/local/gromacs/share/gromacs/top/aminoacids.dat

Group 0 (System) has 99637 elements

Group 1 (Protein) has 8380 elements

Group 2 (Protein-H) has 4263 elements

Group 3 (C-alpha) has 534 elements

Group 4 (Backbone) has 1602 elements

etc.

We are going to choose **System** (group 0), to write all the system as output and hence being coherent with the system topology.

Executing these commands will generate a new trajectory with 20 snapshots (10000/500), named *trajectory.20.xtc*, in **Gromacs XTC** format, ready to be uploaded to **MDWeb** server.

CRD, Binpos, NetCDF, DCD trajectories:

Use *ptraj* from [Ambertools](#) package to reduce the size of a trajectory in **DCD, NetCDF, Binpos or CRD** formats.

Usage: *ptraj structure.top < ptrajReducing.in*

where structure.top is the structure topology in **PRMtop** or **PSF** format, and *ptrajReducing.in* is a file containing the appropriate commands:

```
trajin trajectory.crd 1 10000 500 # Input trajectory, first and last snapshot to read and offset.
trajout trajectory.20.crd # Output trajectory, in Amber ASCII CRD format (ptraj default).
go
```

Executing these commands will generate a new trajectory with 20 snapshots (10000/500), named trajectory.20.crd, in **Amber ASCII CRD** format, ready to be uploaded to **MDWeb** server.

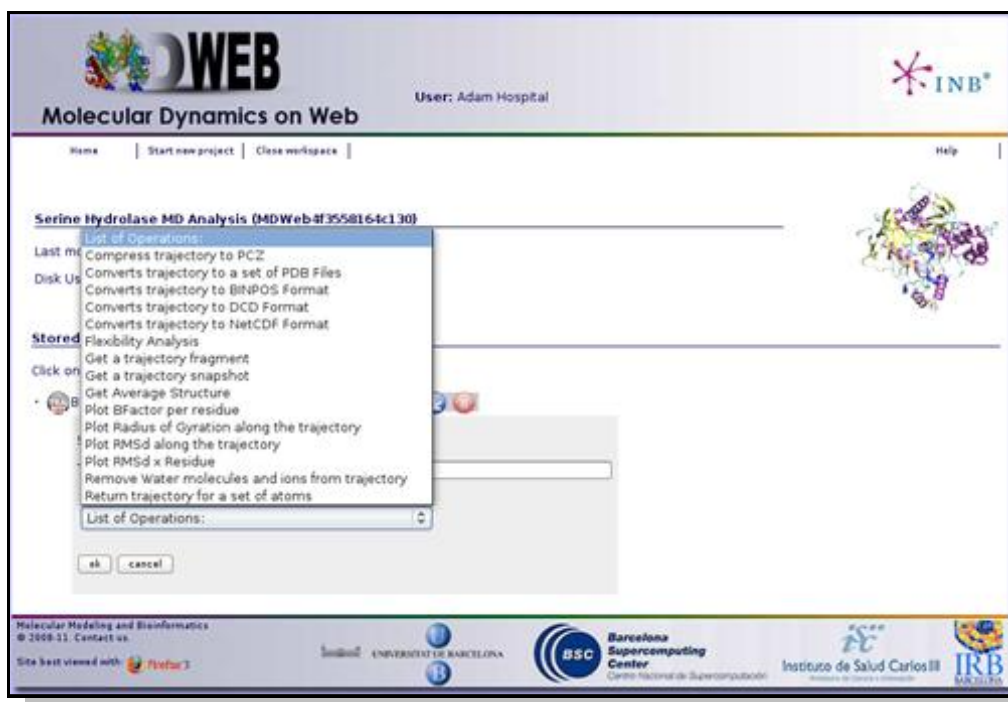
To start our analysis, we are going to put this new generated 20 snapshots trajectory in the **Trajectory File** input box, and the associated topology (the same file used for the molecular dynamics simulation) in the **Topology File** input box.

The screenshot displays the MDWeb web interface. At the top left is the MDWeb logo, and at the top right is the INB logo. The user is identified as 'Adam Hospital'. The main content area shows a project titled 'Serine Hydrolase MD Analysis (MDWeb#f3558164c130)' with a last modification date of '13/02/2012 16:07' and a disk usage of '56.7 MB'. Below this, there is a section for 'Stored structures' with a list item 'Base trajectory (51.5 MB)' marked with a green checkmark. The footer contains logos for Molecular Modeling and Bioinformatics, Universitat de Barcelona, BSC (Barcelona Supercomputing Center), and Instituto de Salud Carlos III.

4. Running Analysis

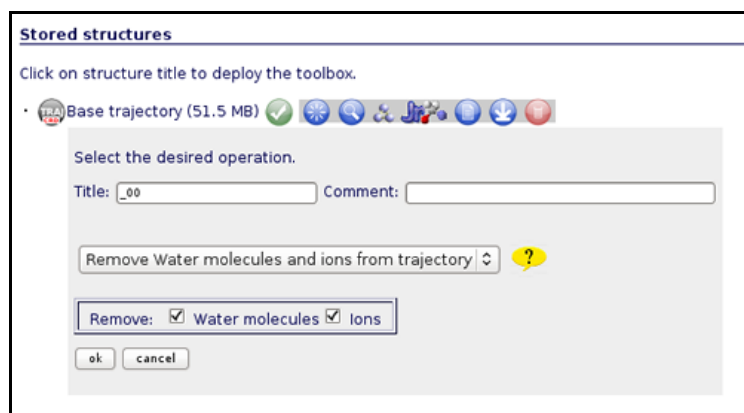
Once we have our trajectory uploaded, we can begin with the analysis. **MDWeb** offers a set of basic analysis that can be divided in 3 different sections:


- Trajectory manipulation: format conversions, slice/snapshot extraction, etc.
- Analysis per Residue/Structure.
- Flexibility Analysis (link to [FlexServ](#)).

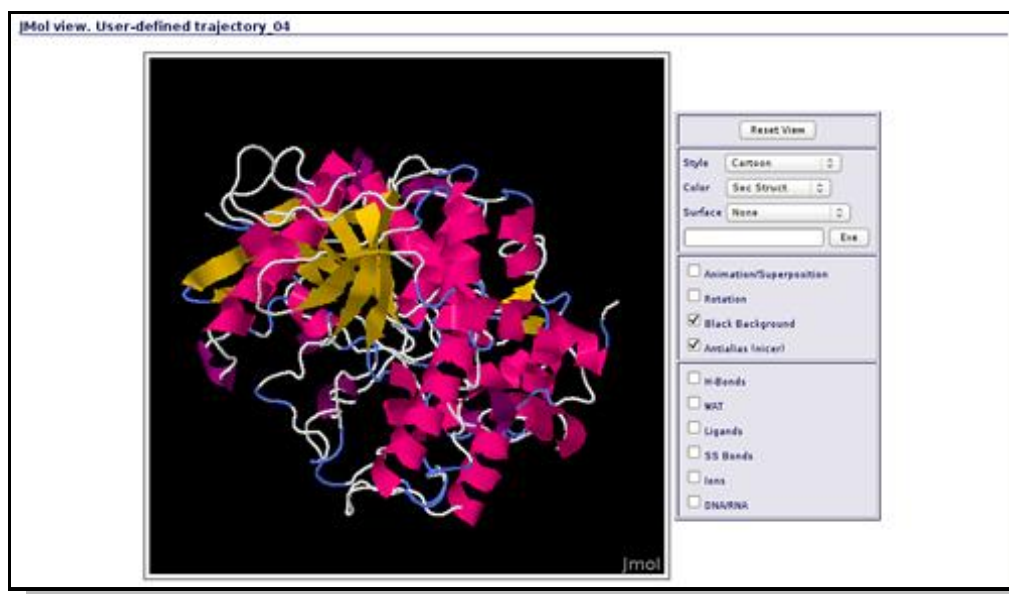


In this specific example we are not interested in converting the trajectory format, but we will begin applying some manipulations to it. The most usual and important one is stripping the solvent, usually together with the counterions, when user is only interested in studying the protein molecule.

To do that, click on the operation called ***Remove water molecules and ions from trajectory***. We can choose whether we would like to remove only water molecules, only counterions or both. In this case, we will remove both, obtaining the trajectory (and the correct topology associated) for just the structure of interest.

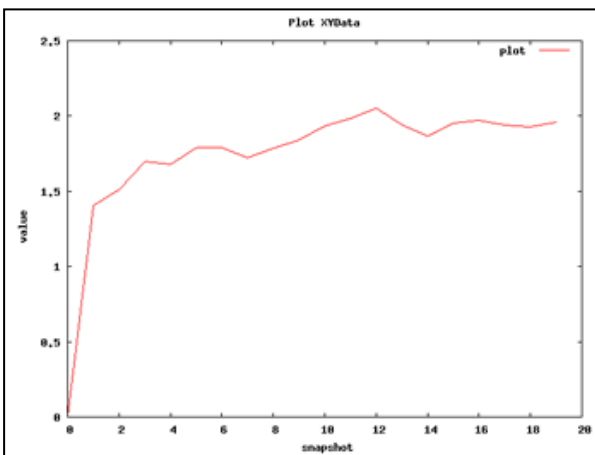
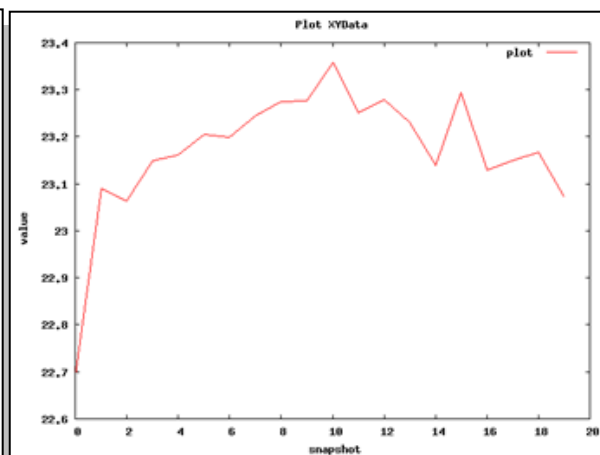


The first noticeable thing once we have the "dry" trajectory, is that it is really smaller in size than the solvated one. That allows the user to animate the trajectory with Jmol applet. If we try to visualize the original solvated structure, MDWeb will show a warning message because the trajectory is too large, recommending to remove solvent. So, clicking at the corresponding Jmol icon , a new window with the Jmol interactive visualizer will be opened. It is a good first approximation to take a look at the dynamics of the structure, before obtaining analysis data.

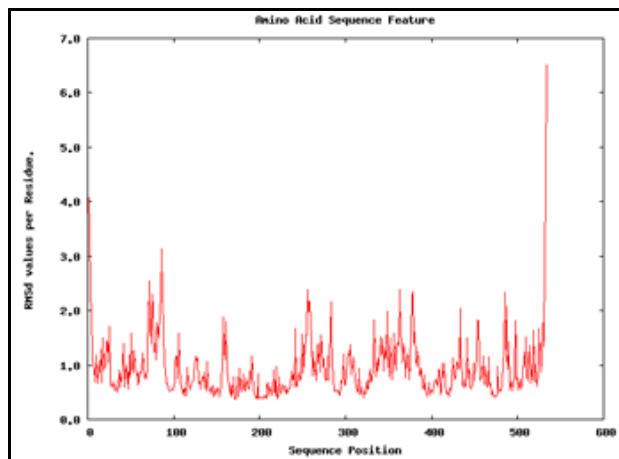
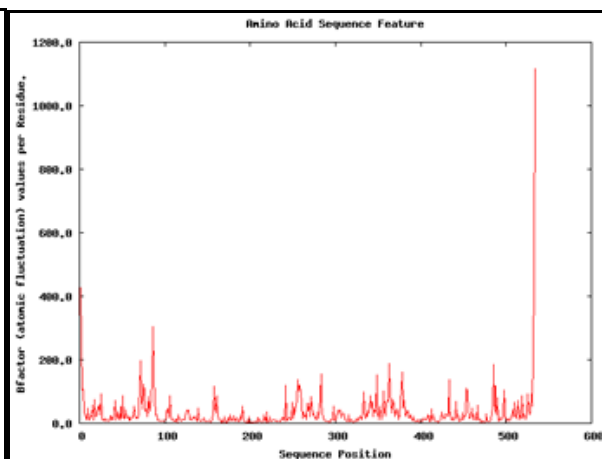


Now we can begin with the basic data analysis. From the list, we can choose two basic analysis as **Root Mean Square deviation** and **Radius of Gyration**. With these two analysis we will be able to see the deviation of the structure during the dynamics, whether it maintains its conformation during the 10 ns length or it suffers some distortion.

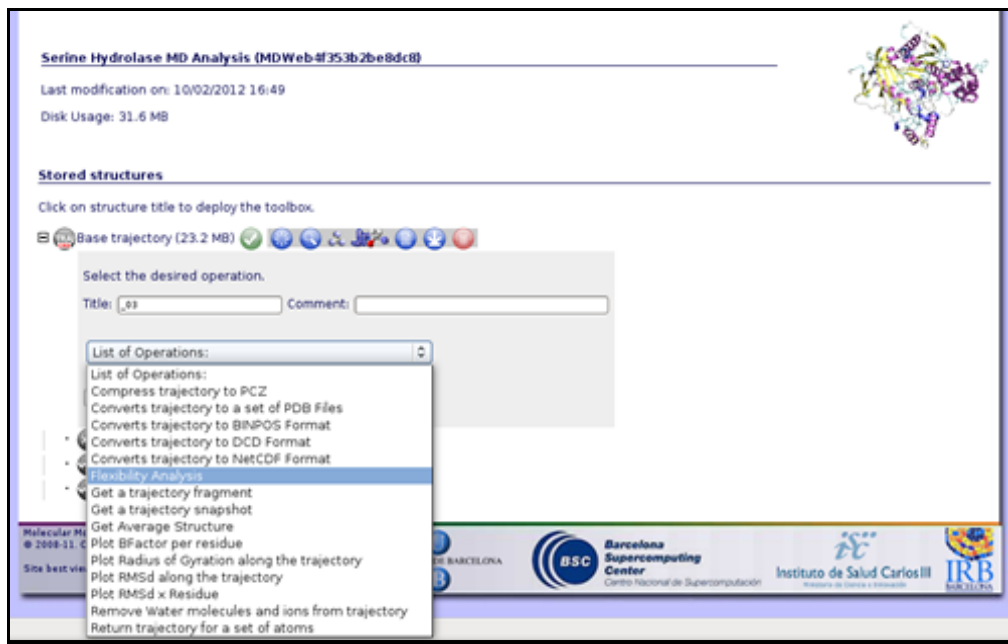
Each of the analysis plot can be visualized clicking at the correspondent icon .

*RMSd Analysis**Radius of Gyration*

We can apply a couple of additional analysis to get a first impression about the flexibility of the structure. These are the **Root Mean Square deviation per Residue** and the **Bfactor per Residue** analyses. Taking a look at the plots, we can easily identify the regions of the structure having more mobility (usually loops) and the regions that are almost kept fixed during the whole simulation.

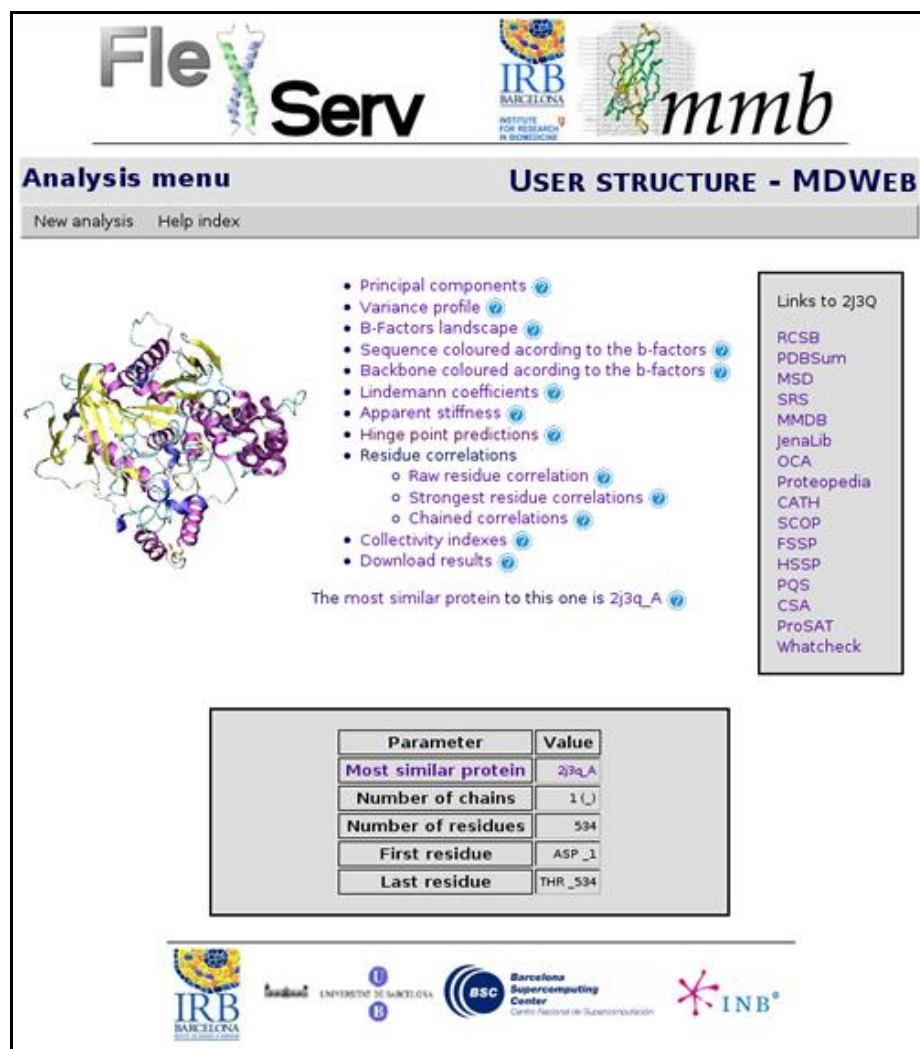
*RMSd x Residue**Bfactor x Residue*



If we are interested in more flexibility analysis, MDWeb offers the possibility to send the project to our flexibility server [FlexServ](#). Just click on the operation called **Flexibility Analysis**.



FlexServ is a server aimed to show in an easy and visual way flexibility-related properties of proteins. It computes a big set of flexibility analysis like:

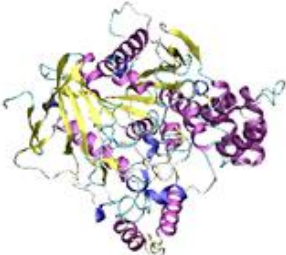
- Principal Components.
- B-factor landscape.
- Lindemann Coefficients.
- Hinge Point Predictions.
- Residue Correlations.
- etc.



FlexServ  

Analysis menu **USER STRUCTURE - MDWEB**

[New analysis](#) [Help index](#)








- [Principal components](#)
- [Variance profile](#)
- [B-Factors landscape](#)
- [Sequence coloured according to the b-factors](#)
- [Backbone coloured according to the b-factors](#)
- [Lindemann coefficients](#)
- [Apparent stiffness](#)
- [Hinge point predictions](#)
- [Residue correlations](#)
 - [Raw residue correlation](#)
 - [Strongest residue correlations](#)
 - [Chained correlations](#)
- [Collectivity indexes](#)
- [Download results](#)

The most similar protein to this one is [2j3q_A](#)

Links to 2j3Q

- [RCSB](#)
- [PDBSum](#)
- [MSD](#)
- [SRS](#)
- [MMDb](#)
- [JenaLib](#)
- [OCA](#)
- [Proteopedia](#)
- [CATH](#)
- [SCOP](#)
- [FSSP](#)
- [HSSP](#)
- [PQS](#)
- [CSA](#)
- [ProSAT](#)
- [Whatcheck](#)

Parameter	Value
Most similar protein	2j3q_A
Number of chains	1 (1)
Number of residues	534
First residue	ASP_1
Last residue	THR_534

So with this set of analysis, we have been able to see that the simulated structure has not suffered critical structural deformations. It has not gone more than 2\AA away from the initial structure, and the **Radius of Gyration** has been also maintained around 20\AA . From the flexibility part, we identified some flexible regions from the **Bfactor** and **RMSd per residue** analysis, that are located mostly in loop regions. We launched a **FlexServ** analysis to obtain more information about these flexible part.