



CREER... CREAR... CRECER

Red BIO-BIO-MOL

Curso de Posgrado: Vistas panorámicas desde el gen hasta la cristalización de una enzima para conocer su función

TUTORIAL

MODELADO COMPARATIVO DE PROTEINAS

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PARA HACER UN MODELADO POR HOMOLOGÍA SE NECESITA:

❁ Una secuencia aminoacídica a modelar. En este tutorial se trabajará con el transportador de amonio de *Pseudomonas aeruginosa* (PA5287)

❁ Una estructura resuelta experimentalmente con secuencia aminoacídica homóloga a la secuencia a modelar. Este modelo debe estar descrito en un archivo PDB, que se obtiene del Protein Data Bank (www.pdb.org)

Nota: Algunos de los archivos obtenidos en este tutorial estarán disponibles para no esperar los resultados. En los archivos que iras generando se sugerirán nombres para que coincidan con los disponibles, pero puedes elegir los nombres que desees.

BUSCAMOS LA SECUENCIA A MODELAR

<http://www.pseudomonas.com/getAnnotation.do?locusID=PA5287>

Pseudomonas Genome Database v2

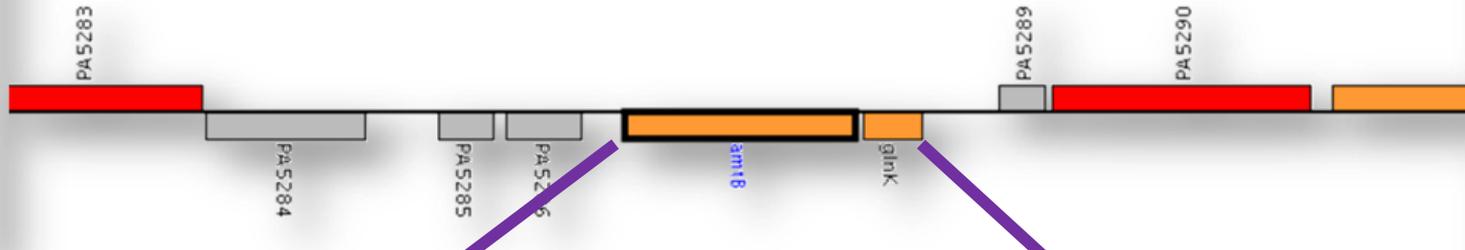
[contact us](#) | [site map](#) | [view my clipboard](#)

Home Database Search Updates Log GBrowse Tools Download About Whats New Links

[Add this annotation to your clipboard](#)

PA5287

[Key to diagram](#)



ammonium
transporter AmtB

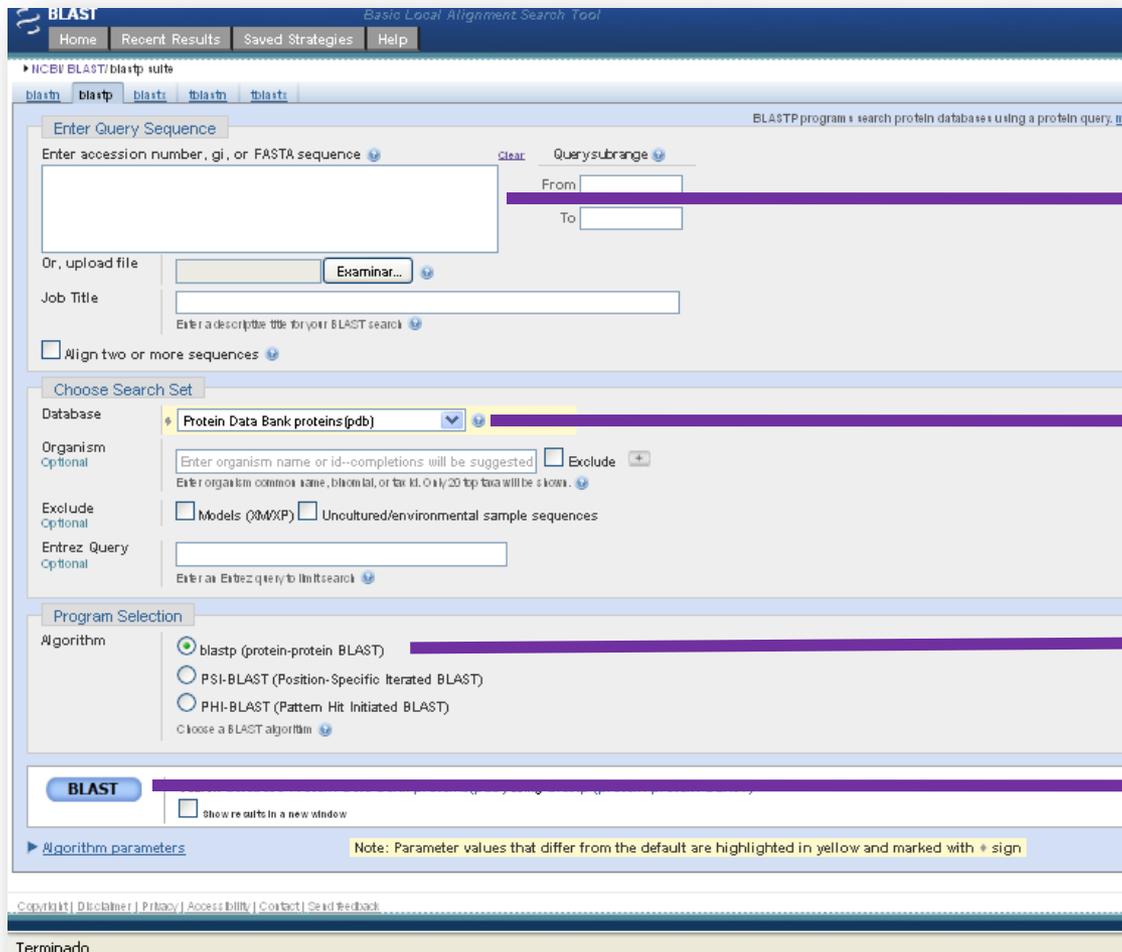
nitrogen regulatory
protein P-II 2

Ambos genes son Clase 2:
Averiguar que significa esto.

BUSCAMOS HOMOLOGOS DE ESTRUCTURA CONOCIDA

- ✿ En la solapa “Sequence data” obtener la secuencia de la proteína
- ✿ Ingresar a la pagina del BLAST (<http://www.ncbi.nlm.nih.gov/BLAST/>)
- ✿ Seleccionar el algoritmo “Protein Blast” y realizar a búsqueda en la base de datos del PDB

BLAST: Basic Local Alignment Search Tool



The screenshot shows the NCBI BLAST web interface. The main form is titled "Enter Query Sequence" and includes a large text input field for the query sequence, a "Clear" button, and a "Query subrange" section with "From" and "To" input fields. Below this is an "Or, upload file" section with a file selection button labeled "Examinar...". There is also a "Job Title" input field and a checkbox for "Align two or more sequences".

The "Choose Search Set" section includes a "Database" dropdown menu set to "Protein Data Bank proteins (pdb)", an "Organism" input field with a search icon, and checkboxes for "Exclude" options: "Models (MMXP)" and "Uncultured/environmental sample sequences". There is also an "Entrez Query" input field.

The "Program Selection" section has three radio buttons: "blastp (protein-protein BLAST)" (selected), "PSI-BLAST (Position-Specific Iterated BLAST)", and "PHI-BLAST (Pattern Hit Initiated BLAST)".

At the bottom, there is a large blue "BLAST" button and a checkbox for "Show results in a new window".

Annotations with purple arrows point to the following elements:

- The "Enter Query Sequence" input field.
- The "Protein Data Bank proteins (pdb)" dropdown menu.
- The "blastp (protein-protein BLAST)" radio button.
- The "BLAST" button.

Ingresar secuencia

Elegir base de datos pdb

Seleccionar algoritmo blastp
(protein-protein BLAST)

Enviar la búsqueda

Ejemplo de resultado:

Protein Sequence (442 letters)

Query ID Id|5201
Description None
Molecule type amino acid
Query Length 442

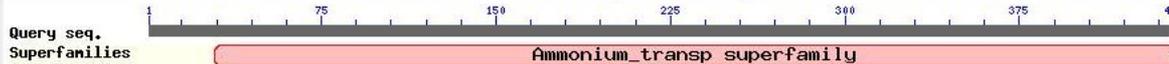
Database Name pdb
Description PDB protein database
Program BLASTP 2.2.24+ [Citation](#)

Other reports: [Search Summary](#) [Taxonomy reports](#) [Distance tree of results](#) [Related Structures](#) [Multiple alignment](#)

Graphic Summary

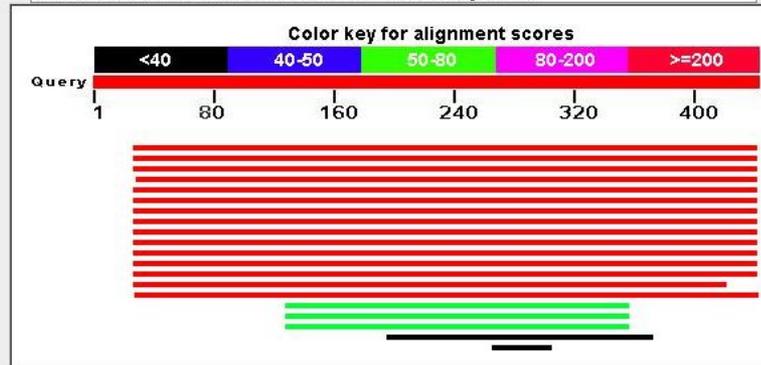
Show Conserved Domains

Putative conserved domains have been detected, click on the image below for detailed results.



Distribution of 20 Blast Hits on the Query Sequence

Mouse-over to show define and scores, click to show alignments



Conserved Domain Database (CDD)

Hits

¿Que significan los diferentes colores?

Analizar:

- ❁ Posee dominios conocidos?
- ❁ Posee homólogos de estructura conocida?
- ❁ Que porcentaje de identidad presenta con los posibles moldes? Permite realizar modelado comparativo?
- ❁ ¿Existe mas de un posible molde? Si es así, ¿Que criterios tendrías en cuenta para seleccionar la proteína molde?



Una vez elegido el molde, acceder al banco de datos del Protein Data Bank y buscar la anotacion de dicho molde:

<http://www.pdb.org/pdb/home/home.do>

Molde: 2NS1

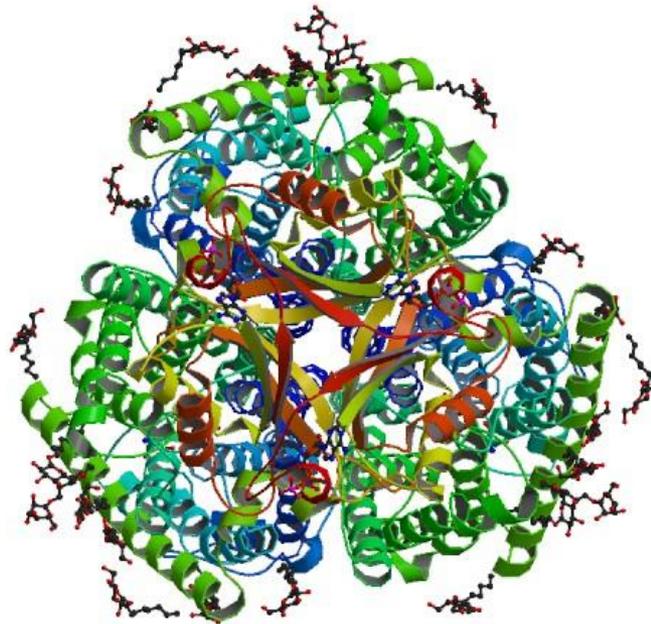
Inhibitory complex of the transmembrane ammonia channel, AmtB, and the cytosolic regulatory protein, GlnK, at 1.96 Å.



Chain A: Ammonia channel



Chain B: Nitrogen regulatory protein P-II 2



Analizar la estructura:

A que organismo pertenece?

Como esta compuesto este complejo?

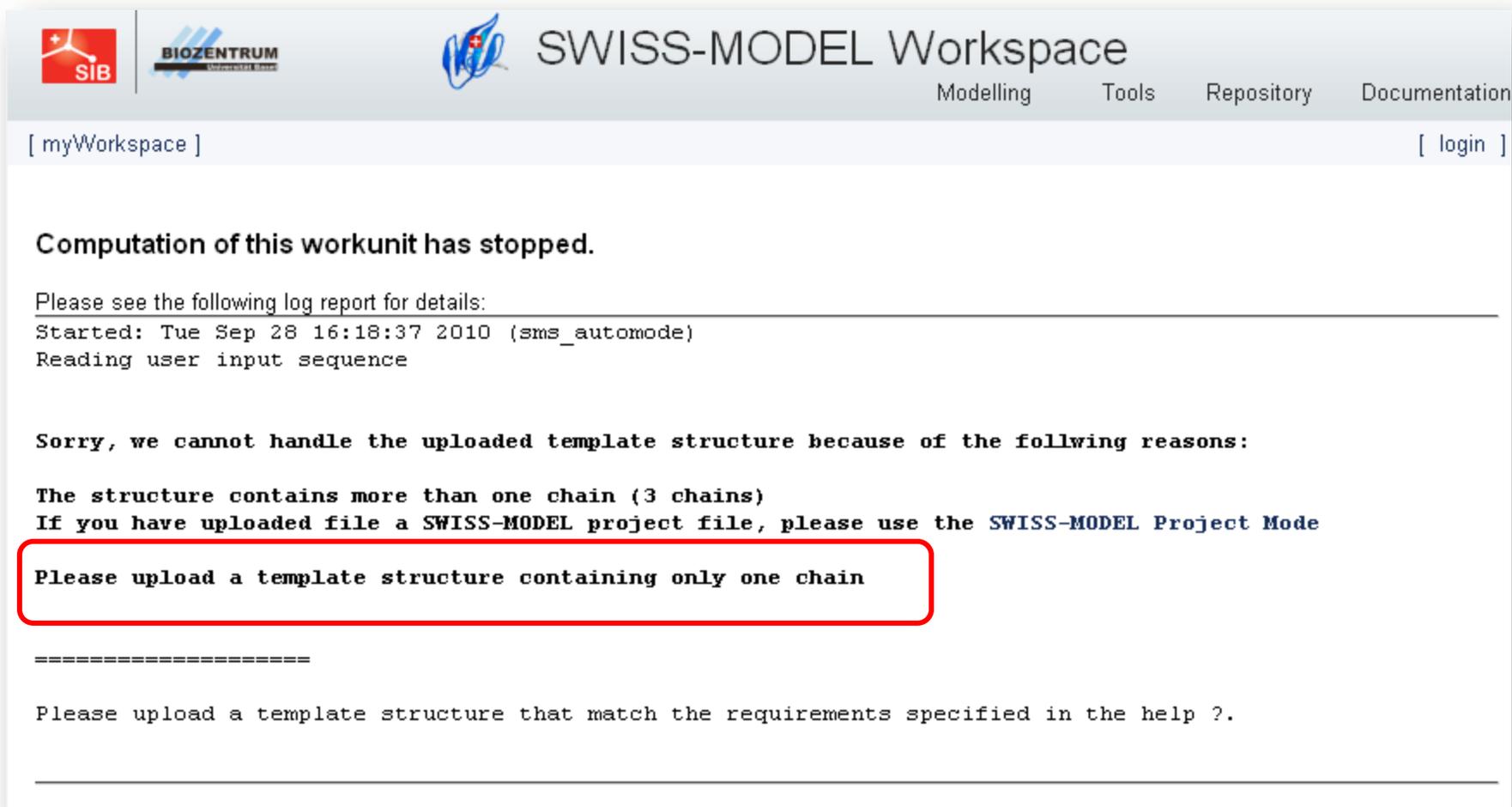


Acceder al SWISS-MODEL Workspace
<http://swissmodel.expasy.org/workspace/index.php?>

The screenshot shows the SWISS-MODEL Workspace website. At the top left, there are logos for SIB (Swiss Institute of Bioinformatics) and BIOZENTRUM. The main header features the SWISS-MODEL Workspace logo, which is a blue ribbon structure with a red Swiss cross, and the text 'SWISS-MODEL Workspace'. Below the header, there are navigation links for 'Modelling', 'Tools', 'Repository', and 'Documentation'. A user session indicator '[myWorkspace]' is visible on the left, and a '[login]' link is on the right. The main content area displays the SWISS-MODEL Workspace logo and the text 'SWISS-MODEL Workspace' and 'An Automated Comparative Protein Modelling Environment'. At the bottom, it states 'SIB - Biozentrum Basel site provided by:' followed by the logos for BIOZENTRUM and SIB (Swiss Institute of Bioinformatics).

Pueden crear su propia cuenta, sino se les suministrara una cuenta en el desarrollo del TP

No es posible modelar polímeros. Debemos modelar el monómero y luego ensamblar el trómero



The screenshot shows the SWISS-MODEL Workspace interface. At the top, there are logos for SIB, BIOZENTRUM, and SWISS-MODEL. The main navigation bar includes links for Modelling, Tools, Repository, and Documentation. Below the navigation bar, there is a user session indicator [myWorkspace] and a [login] link. The main content area displays an error message: "Computation of this workunit has stopped." followed by a log report. The log report indicates that the computation started on Tue Sep 28 16:18:37 2010 in sms_automode and was reading user input sequence. The error message states: "Sorry, we cannot handle the uploaded template structure because of the following reasons: The structure contains more than one chain (3 chains) If you have uploaded file a SWISS-MODEL project file, please use the SWISS-MODEL Project Mode Please upload a template structure containing only one chain". The last sentence is highlighted with a red box. Below the error message, there is a separator line and a final instruction: "Please upload a template structure that match the requirements specified in the help ?."

[myWorkspace] [login]

Computation of this workunit has stopped.

Please see the following log report for details:

Started: Tue Sep 28 16:18:37 2010 (sms_automode)
Reading user input sequence

Sorry, we cannot handle the uploaded template structure because of the following reasons:

The structure contains more than one chain (3 chains)
If you have uploaded file a SWISS-MODEL project file, please use the SWISS-MODEL Project Mode

Please upload a template structure containing only one chain

=====

Please upload a template structure that match the requirements specified in the help ?.



En la solapa Automate mode, enviar el proyecto

The screenshot shows the SWISS-MODEL Workspace interface. At the top, there are logos for SIB, BIOZENTRUM, and SWISS-MODEL. The main header reads "SWISS-MODEL Workspace" with sub-menus for "Modelling" and "Tools". A dropdown menu is open under "Modelling", showing options: "myWorkspace", "Automated Mode" (highlighted in red), "Alignment Mode", and "Project Mode". Below this, the page title is "[myWorkspace]" and the main heading is "SwissModel Automatic Modelling Mode" with a red question mark icon. There are input fields for "Email:" and "Project Title:". A large purple arrow points to the right with the text "Ingresar secuencia". Below that is a "Submit Modelling Request" button. At the bottom, under "Advanced options:", there are fields for "Use a specific template:" (with a red question mark icon), "PDB-ID:" (containing "2NS1"), and "Chain:" (containing "A"). A purple arrow points to the right from the "Chain:" field with the text "Especificar molde".

Así se verá la pantalla del workspace

The screenshot shows the SWISS-MODEL Workspace interface. At the top, there are logos for SIB and BIOZENTRUM. The main header reads "SWISS-MODEL Workspace" with navigation links for "Modelling", "Tools", "Repository", and "Documentation". Below the header, there is a user profile section for "[myWorkspace]" with links for "[Settings]" and "[logout]".

The main content area is titled "Workspace" and contains a table of workunits. The table has columns for "Workunit", "Type", "Title", and "Status". The workunits listed are:

Workunit	Type	Title	Status
P000007	Modelling - Project Mode	amtB	finished
P000010	Modelling - Project Mode	2	finished
P000013	Modelling - Automated Mode	auto	finished
P000014	Modelling - Automated Mode		finished
P000016	Modelling - Automated Mode	Con_2NS1_A	7 days left
P000017	Modelling - Automated Mode	glnK_2NS1_B	1 days left

Below the table, there is a "Symbols:" section with a legend:

- submission not finished (green circle with exclamation mark)
- queued (grey circle with exclamation mark)
- running (blue circle with exclamation mark)
- failed/stopped (red circle with exclamation mark)
- finished (green checkmark)
- 7 days left (green circle with exclamation mark)
- 1 days left (red circle with exclamation mark)
- will be deleted (red circle with exclamation mark)
- keep 7 days longer (blue circle with exclamation mark)
- delete workunit (red circle with exclamation mark)

Estado del proyecto

Tiempo de permanencia que le restan al proyecto en el workspace.
(Por defecto se mantienen 7 días, pero este plazo puede extenderse)

Workunit: P000032 Title: paAmtB_2



Go to: [Template Selection] [Alignment] [Modelling Log] [Evaluation]

Model Details: Segment 1



Model info:

modelled residue range: 27 to 441
based on template: **2ns1A** (1.96 Å) **Remarks:** No search for template was performed.
Only user-specified template was used for modelling.
Sequence Identity [%]: 50.839
Evaluate: 0.00e-1

display model: as pdb - as DeepView project
download model: as pdb - as Deepview project - as text

Resultado de la evaluación

Información del modelado

Alineamiento

Descargar el modelo en formato “pdb”

(para ganar tiempo, estos archivos serán suministrados: Model_AmtB.pdb)

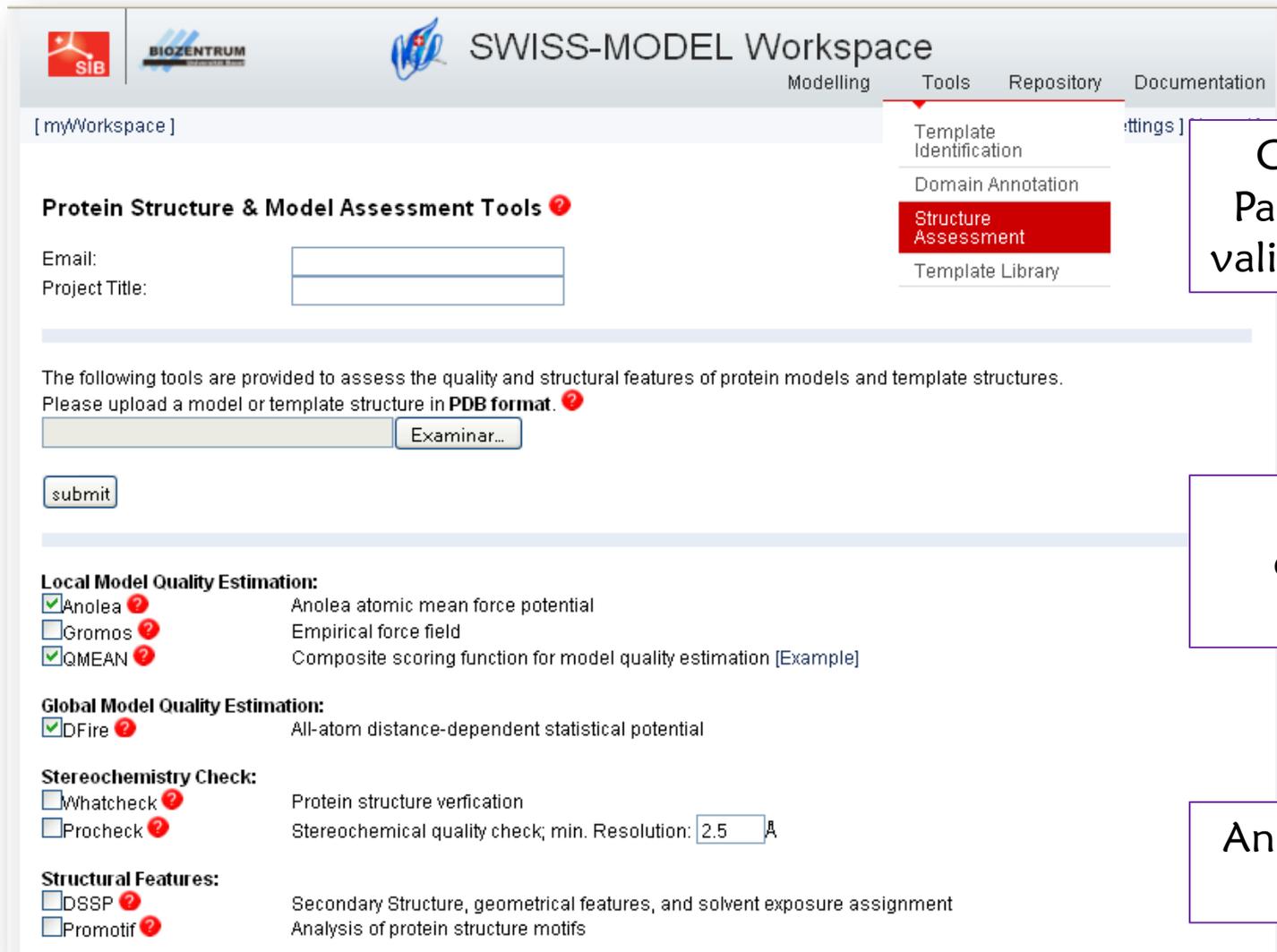


Analizar:

- ✿ Alineamiento: hay zonas problemáticas?
- ✿ Es buena la energía del modelo?
- ✿ Analizar la calidad del modelo con las funciones ANOLEA y GROMOS: hay zonas problemáticas?

Ya tenemos el modelo, ahora hay que validarlo

Tools → structure assessment



SWISS-MODEL Workspace
Modelling Tools Repository Documentation

[myWorkspace]

Protein Structure & Model Assessment Tools ?

Email:
Project Title:

The following tools are provided to assess the quality and structural features of protein models and template structures.
Please upload a model or template structure in **PDB format**. ?

Local Model Quality Estimation:

- Anolea ? Anolea atomic mean force potential
- Gromos ? Empirical force field
- QMEAN ? Composite scoring function for model quality estimation [Example]

Global Model Quality Estimation:

- DFire ? All-atom distance-dependent statistical potential

Stereochemistry Check:

- Whatcheck ? Protein structure verification
- Procheck ? Stereochemical quality check; min. Resolution: Å

Structural Features:

- DSSP ? Secondary Structure, geometrical features, and solvent exposure assignment
- Promotif ? Analysis of protein structure motifs

Otros parámetros
Para la evaluación y
validación del modelo



Validación
estereoquímica:
PROCHECK



Analizar el gráfico de
Ramachandran

Muy Bien!!! En este punto, hemos construido y validado el modelo del transportador de amonio AmtB de *P. aeruginosa*. Pero la unidad funcional es un trímero, ahora debemos ensamblar los monómeros para obtener el trímero.



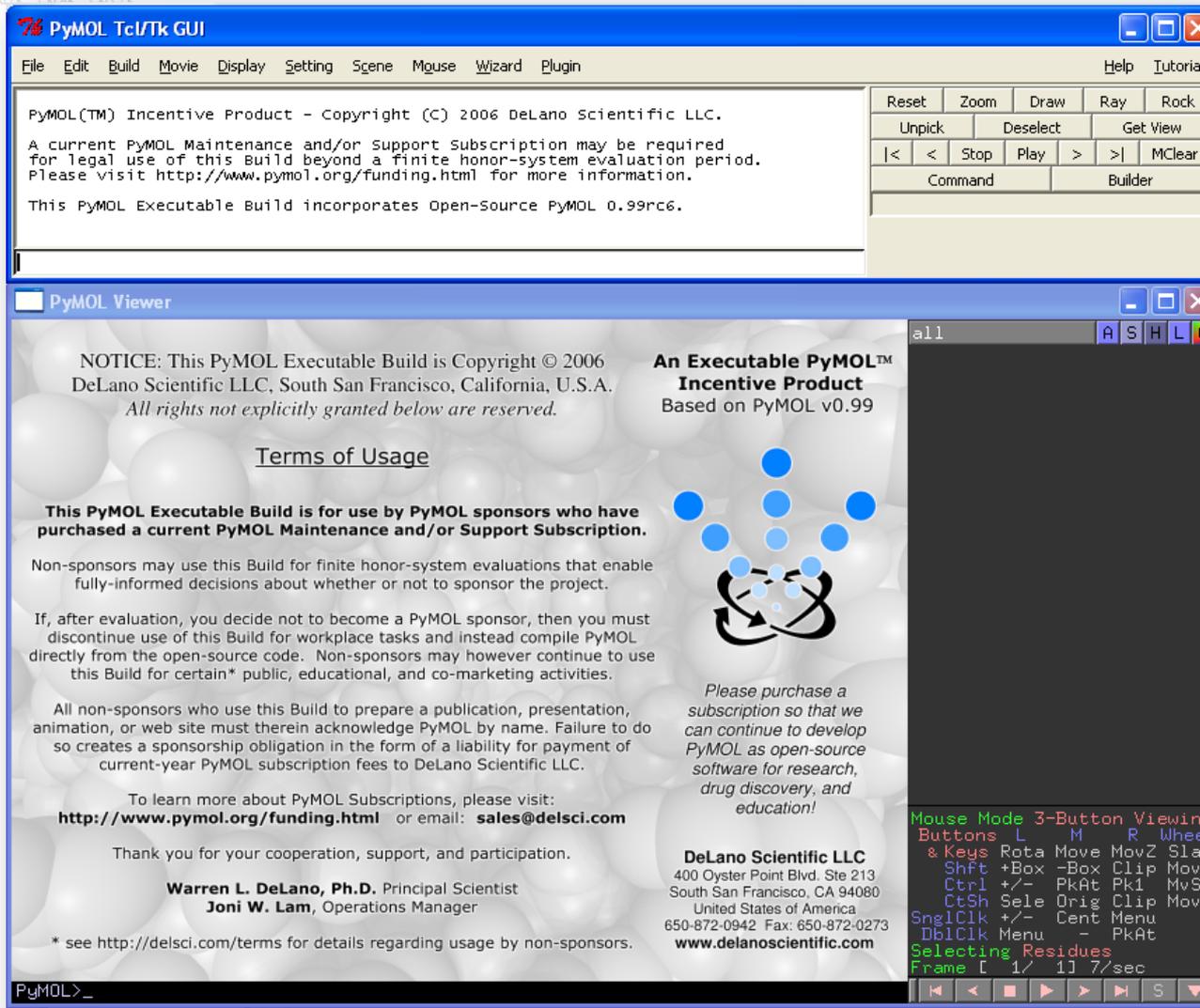
PyMOL (versión Educativa)

<http://pymol.org/edu/>

VMD

<http://www.ks.uiuc.edu/Research/vmd/>

En este Trabajo Practico emplearemos PyMOL



PyMOL Tcl/Tk GUI

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help Tutorial

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Reset Zoom Draw Ray Rock
 Unpick Deselect Get View
 < < Stop Play > > MClear
 Command Builder

PyMOL Viewer

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Warren L. DeLano, Ph.D. Principal Scientist
Joni W. Lam, Operations Manager

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all A S H L C

Mouse Mode 3-Button Viewing
 Buttons L M R Wheel
 & Keys Rota Move MovZ Slab
 ShFt +Box -Box Clip MovS
 Ctrl +/- PkAt Pk1 MovSZ
 CtSh Sele Orig Clip MovZ
 SnglClk +/- Cent Menu
 DblClk Menu - PkAt
 Selecting Residues
 Frame [1/ 1] 7/sec

PyMOL>_

Consola de comandos

A: action
 S: show
 H: hide
 L: label
 C: color

Visor de moléculas

En primer lugar debemos buscar la estructura de la unidad biológica, ya que la molécula que usamos hasta el momento (2NS1) solo tiene las coordenadas atómicas de un monómero de cada proteína

En la pagina del Protein Data Bank, busca nuevamente la entrada para 2NS1, y accede a la solapa links

Accede a PDBSum. Esta es una base de datos del Instituto Europeo de Bioinformática de Inglaterra (EBI) que nuclea mucha de la información disponible para la estructura buscada

Al margen derecho, en el menu “Quick links” acceder a PQS (Protein Quaternary Structure Server). Descargar la estructura trimerica como formato pdb. Aquí la nombraremos 2NS1_trimero.pdb

EMBL-EBI EB-eye Search All Databases Enter Text Here Go Reset Advanced Search Give us feedback

Databases Tools EBI Groups Training Industry About Us Help Site Index

PDBsum Go to PDB code: 2ns1 go

Top page Protein Ligands Prot-prot Clefs Links

Transport protein/signaling protein PDB id **2ns1**

Main view

Right view

Bottom view

Quick links

- [RCSB](#)
- [PDBe](#)
- [SRS](#)
- [MMDB](#)
- [JenaLib](#)
- [OCA](#)
- [PDBWiki](#)
- [Proteopedia](#)
- [CATH](#)
- [SCOP](#)
- [FSSP](#)
- [HSSP](#)
- [PDBSWS](#)
- [OPM](#)
- [PQS](#)
- [ProSAT](#)
- [Whatcheck](#)
- [EDS](#)

Protein Quaternary Structure Server

Procheck

Clefts

Contents

- Description**
 - Header details
 - Header records
 - References
 - PROCHECK
- Protein chains**
 - A 404 a.a. *
 - B 113 a.a. *
- Ligands**
 - BOG x8
 - TRS x2

PDB id: 2ns1
Name: Transport protein/signaling protein
Title: Crystal structure of the e. Coli ammonia channel amtB complexed with the signal transduction protein glk
Structure: Ammonia channel. Chain: a. Fragment: residues 23-428. Synonym: ammonia transporter. Engineered: yes. Nitrogen regulatory protein p-ii 2. Chain: b. Engineered: yes. Mutation: yes
Source: Escherichia coli k12. Organism_taxid: 83333. Strain: k12. Gene: amtB. Expressed in: escherichia coli. Expression_system_taxid: 562. Gene: glk. Expressed in: escherichia coli bl21(de3). Expression_system_taxid: 469008.
UniProt: Chain A: P69681 (AMTB_ECOLI)

Seq: Ammonia channel

Encontrar: id Siguiente Anterior Resaltar todo Coincidencia de mayúsculas/minúsculas

Terminado

PQS OUTPUT - Mozilla Firefox

Archivo Editor Ver Historial Marcadores Herramientas Ayuda

http://www.ebi.ac.uk/pdbe/pqs/pqs-bin/macmol.pl?filename=2ns1

protein data bank

Ahora: Predominio de nubes, 14° C

Jue: 20° C

Vie: 23° C

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MacroMolecular File retrieval:
See the [Documentation](#) for a description of method used to automatically generate these files

Likely Quaternary Structure or MacroMolecular Assembly:
(This is often, but not necessarily the Biological Unit)

- Click on this button along side each filename to get a rasmol view

The Biological relevant molecule for **2ns1** can be assembled from the contents of the deposited coordinates by the application of crystallographic symmetry operations to give a MacroMolecule of type **HEXAMERIC**. The MacroMolecule can be downloaded as the following file:

Rasmol [2ns1_mmol](#) (file size in bytes: 932085)

Other files:

- [2ns1_rem350](#) file rem350 h

Test for Crystal Packing:

The Oligomeric state given h
Structure 2ns1 has:

- 4 residues exposed in an iso
- 6 interchain salt bridges within the complex
- shows a loss of **4091.0 Ang**2** of solvent accessible surface area upon complex formation
- shows a gain in Solvation free energies of folding from isolated chains to the complex of **-249.98 kcal/mol**

Details concerning the results are given in the file [2ns1](#)

[asa Notes](#) Description of method used to differentiate between Crystal Packing and true oligomeric state

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Encontrar: Coincidencia de mayúsculas/minúsculas

Terminado

Descargar la estructura trimerica (se proporcionará: 2NS1_trimero.pdb)

🌸 Cargar la unidad biológica del molde: 2NS1_trimero.pdb

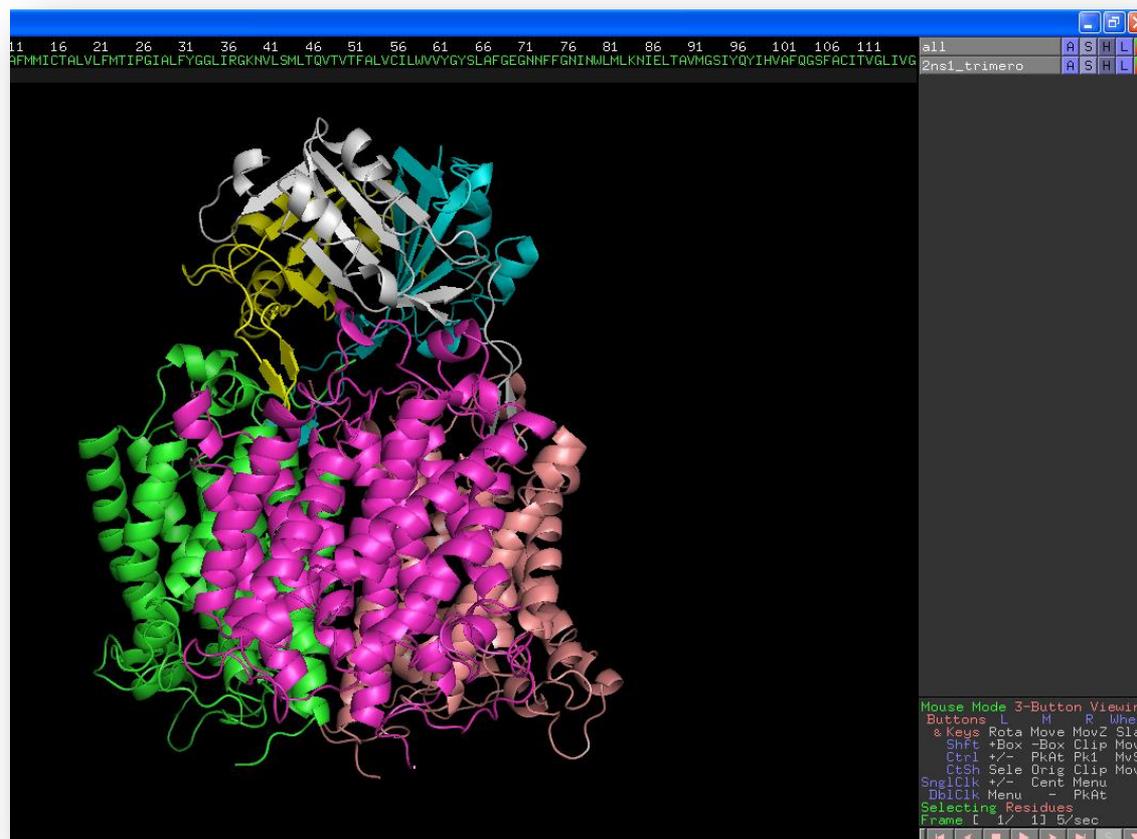
File → *open*

🌸 Representar en cartoon, colorear por cadena

Hide → *everything*

Show → *cartoon*

Color → *by chan* → *by chain*





✿ Crear una selección para cada monómero de AmtB, y renombrarla
(en el trímero, corresponde a cadenas A, C y E).

Pintar los residuos a seleccionar, se crea automáticamente la selección "sele".

Actions → rename selection

✿ Abrir el archivo correspondiente al modelo, representar en cartoon
coloreado por cadena

File → Open

Hide → everything

Show → cartoon

color → by chain → by chain

✿ Duplicar el objeto del modelo 2 veces, de modo de contar con 3
copias. Opcionalmente puede renombrar las copias.

Actions → duplicate object

Actions → rename object

✿ Finalmente se obtiene un sistema como se muestra a continuación



2Ns1_trimero
3 copias del modelo

Monómeros seleccionados

PyMOL Viewer

```

/2ns1_trimero//A/3 6 11 16 21 26 31 36 41 46 51 56 61 66 71 76 81 86 91 96 101 106
AVADKADNAFMMICTALVLFMTIPGIALFYGGILRGKNVLSMLTQVTVFALVCILWVYGYSLAFGEGNFFGNINWMLMKNIELTAVMGSIIYQYIHVAFQGSFACITV
/Model_AmtB/// 27 31 36 41 46 51 56 61 66 71 76 81 86 91 96 101 106 111 116 121 126 131
PVLNSGDTAWMLISTALVLLMTIPGLALFYGGMWRKKNVLSIMMOCFAITGLITILWVYGYSLAFDTAGMEKGVLFNFSFVGGLDKAFLSGLTADGLTSATALFPESVF
/Model_AmtB_chainB/// 27 31 36 41 46 51 56 61 66 71 76 81 86 91 96 101 106 111 116 121 126 131
PVLNSGDTAWMLISTALVLLMTIPGLALFYGGMWRKKNVLSIMMOCFAITGLITILWVYGYSLAFDTAGMEKGVLFNFSFVGGLDKAFLSGLTADGLTSATALFPESVF
/Model_Amt_chainC/// 27 31 36 41 46 51 56 61 66 71 76 81 86 91 96 101 106 111 116 121 126 131
PVLNSGDTAWMLISTALVLLMTIPGLALFYGGMWRKKNVLSIMMOCFAITGLITILWVYGYSLAFDTAGMEKGVLFNFSFVGGLDKAFLSGLTADGLTSATALFPESVF
  
```

all	A	S	H	L	C
2ns1_trimero	A	S	H	L	C
(chainA)	A	S	H	L	C
(chainB)	A	S	H	L	C
(chainC)	A	S	H	L	C
Model_AmtB	A	S	H	L	C
Model_AmtB_chain	A	S	H	L	C
Model_Amt_chainC	A	S	H	L	C

```

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DBlClk Menu - PkAt
Selecting Residues
Frame [ 2 / 2 ] 3/sec
  
```

PyMOL>_

✿ Alinear cada uno de los 3 objetos correspondientes al modelo con la selección correspondiente.

Model_AmtB: Action → align → to selection → chainA

Model_AmtB_chainB: Action → align → to selection → chainB

Model_AmtB_chainC: Action → align → to selection → chainC

✿ De este modo se posicionan las 3 copias del modelo superpuestas con el trímero. Ocultar 2NS1 y se vera el trímero del modelo como se muestra a continuación



PyMOL Viewer

```
CREEE  
/Model_AmtB///27 31 36 41 46 51 56 61 66 71 76 81 86 91 96 101 106 111 116 121 126 131  
PVLNSGDTAWMLISTALVLLMTIPGLALFYGGMVRRAKNVLSIMMQCFAITGLITILWVVYGYSLAFDTAGMEKGVLFNFSFVGGLDKAFLSGLTADGLTSATALFPESVFI  
/Model_AmtB_chainB///27 31 36 41 46 51 56 61 66 71 76 81 86 91 96 101 106 111 116 121 126 131  
PVLNSGDTAWMLISTALVLLMTIPGLALFYGGMVRRAKNVLSIMMQCFAITGLITILWVVYGYSLAFDTAGMEKGVLFNFSFVGGLDKAFLSGLTADGLTSATALFPESVFI  
/Model_Amt_chainC///27 31 36 41 46 51 56 61 66 71 76 81 86 91 96 101 106 111 116 121 126 131  
PVLNSGDTAWMLISTALVLLMTIPGLALFYGGMVRRAKNVLSIMMQCFAITGLITILWVVYGYSLAFDTAGMEKGVLFNFSFVGGLDKAFLSGLTADGLTSATALFPESVFI
```

all	A	S	H	L	C
2ns1_trimero	A	S	H	L	C
(chainA)	A	S	H	L	C
(chainB)	A	S	H	L	C
(chainC)	A	S	H	L	C
Model_AmtB	A	S	H	L	C
Model_AmtB_chain	A	S	H	L	C
Model_Amt_chainC	A	S	H	L	C

Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box ~Box Clip MovS
Ctrl +/- PKAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DbiClk Menu - PkAt
Selecting Residues
Frame [2 / 21 6/sec

PyMOL>_

✿ Grabar cada monómero por separado con formato pdb
File → *save molecule* → (elegir molécula) → *OK* → (elegir destino) → *Guardar*
 (Model_AmtB_chainA, Model_AmtB_chainB y Model_AmtB_chainC)

✿ Abrir los archivos de los monómeros con editor de texto.

✿ Copiar toda la información del monómero B y pegarla debajo del monómero A, con cuidado de mantener la expresión “TER”

✿ Repetir lo mismo para el monómero C de modo de tener un solo archivo con las coordenadas atómicas del trímero.

✿ Modificar manualmente el archivo agregando una columna donde indicar cadenas A, B y C. Guardar en formato pdb (paAmtB.pdb)

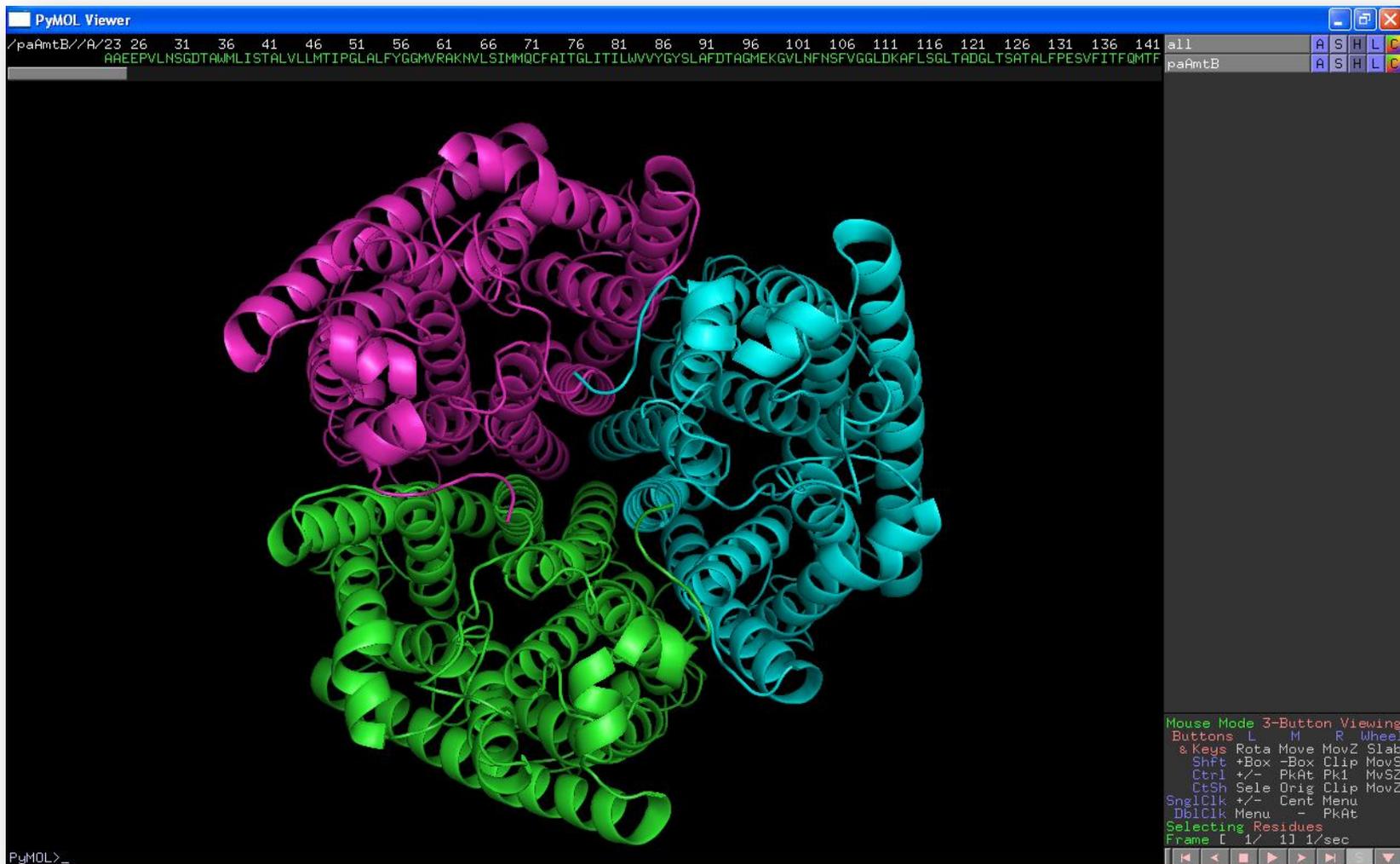
Esta es una tarea lenta y tediosa pero necesaria. Se suministrara el archivo final: paAmtB.pdb

4	ATOM	4	O	ALA	23	5.408	45.1
5	ATOM	5	CB	ALA	23	5.269	43.4
6	ATOM	6	N	ALA	24	6.248	46.0
7	ATOM	7	CA	ALA	24	7.204	46.9
8	ATOM	8	C	ALA	24	6.572	48.3
9	ATOM	9	O	ALA	24	7.221	49.2
10	ATOM	10	CB	ALA	24	8.426	47.1
11	ATOM	11	N	GLU	25	5.297	48.4
12	ATOM	12	CA	GLU	25	4.512	49.6
13	ATOM	13	C	GLU	25	4.373	49.7
14	ATOM	14	O	GLU	25	4.205	48.6
15	ATOM	15	CB	GLU	25	3.159	49.5
16	ATOM	16	CG	GLU	25	2.245	50.7
17	ATOM	17	CD	GLU	25	1.635	50.8
18	ATOM	18	OE1	GLU	25	1.412	49.7
19	ATOM	19	OE2	GLU	25	1.455	51.9
20	ATOM	20	N	GLU	26	4.440	50.9
21	ATOM	21	CA	GLU	26	4.302	51.1
22	ATOM	22	C	GLU	26	3.485	52.4
23	ATOM	23	O	GLU	26	3.671	53.4
24	ATOM	24	CB	GLU	26	5.683	51.2
25	ATOM	25	CG	GLU	26	6.537	52.4
26	ATOM	26	CD	GLU	26	7.901	52.4



3054	ATOM	3054	CD1	TYR	440	9.228	63.2
3055	ATOM	3055	CD2	TYR	440	1.997	61.6
3056	ATOM	3056	CE1	TYR	440	2.367	62.9
3057	ATOM	3057	CE2	TYR	440	1.132	61.3
3058	ATOM	3058	CZ	TYR	440	1.317	62.0
3059	ATOM	3059	OH	TYR	440	0.477	61.8
3060	ATOM	3060	N	ASN	441	7.344	63.3
3061	ATOM	3061	CA	ASN	441	8.333	63.6
3062	ATOM	3062	C	ASN	441	8.415	65.1
3063	ATOM	3063	O	ASN	441	7.928	65.9
3064	ATOM	3064	CB	ASN	441	9.706	63.0
3065	ATOM	3065	CG	ASN	441	9.635	61.5
3066	ATOM	3066	ND2	ASN	441	9.597	61.2
3067	ATOM	3067	OD1	ASN	441	9.535	60.7
3068	TER	3068	OXT	ASN	441	8.917	65.5
3069	ATOM	1	N	ALA	B 23	17.303	81.4
3070	ATOM	2	CA	ALA	B 23	17.615	82.6
3071	ATOM	3	C	ALA	B 23	16.436	83.1
3072	ATOM	4	O	ALA	B 23	16.523	83.1
3073	ATOM	5	CB	ALA	B 23	18.028	83.8
3074	ATOM	6	N	ALA	B 24	15.302	83.3
3075	ATOM	7	CA	ALA	B 24	14.054	83.7
3076	ATOM	8	C	ALA	B 24	13.196	82.5
3077	ATOM	9	O	ALA	B 24	12.097	82.6
3078	ATOM	10	CB	ALA	B 24	13.271	84.7

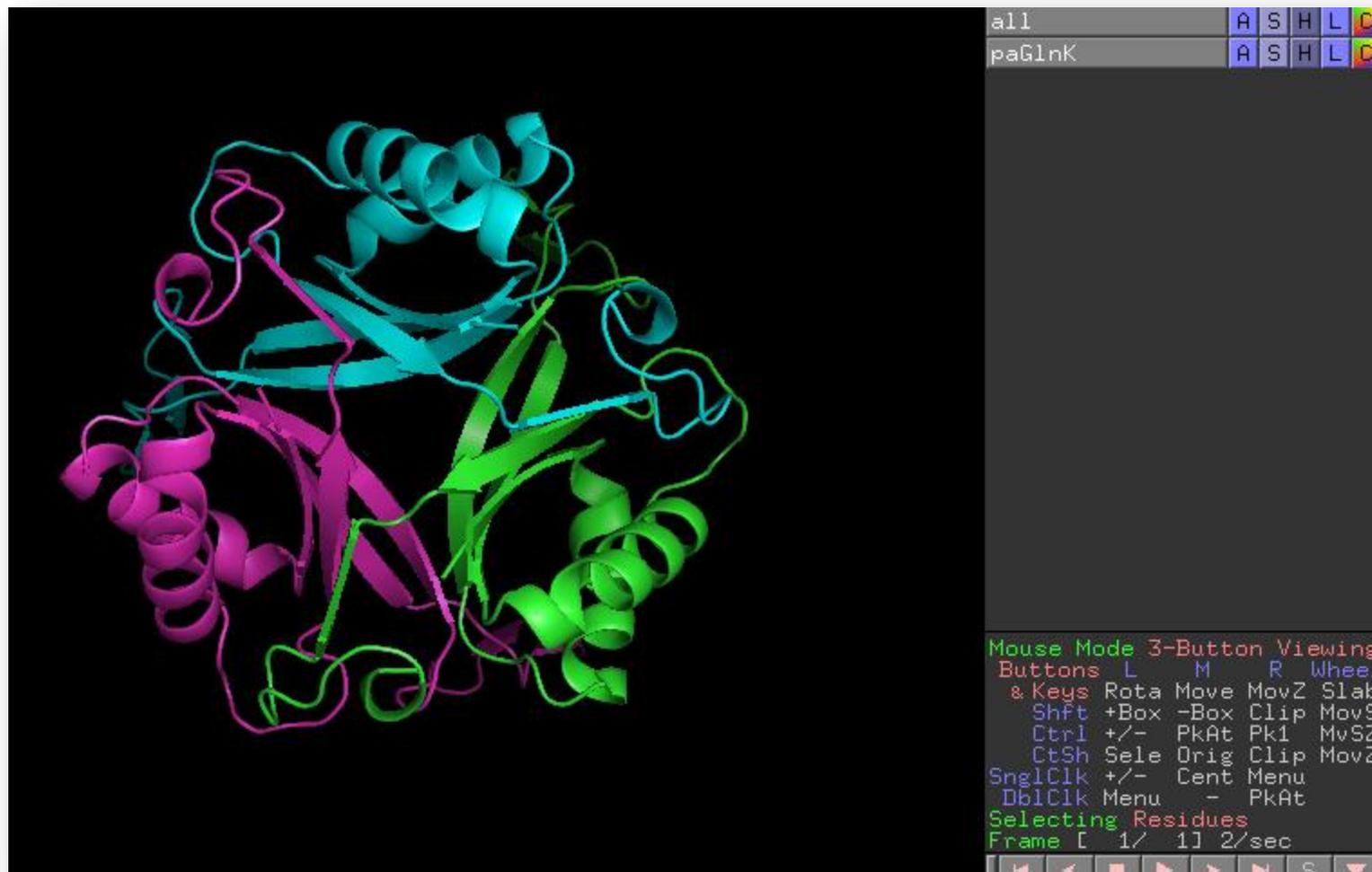
Listo el modelo del trímero del transportador AmtB de *Pseudomonas aeruginosa*!



Te animas a....

- ✿ Modelar la proteína reguladora GlnK
- ✿ Ensamblar el trímero de la proteína regulatoria GlnK
- ✿ Ensamblar el hexámero AmtB-GlnK de *P. aeruginosa*

Modelo del unidad biológica de GlnK de *Pseudomonas aeruginosa*



Modelo del complejo AmtB- GlnK de *Pseudomonas aeruginosa*

