

Tutorial Actividad Práctica 1.4

Modelado estructural de proteínas

The logo consists of the lowercase letters "viu" in white, sans-serif font, centered within a solid orange rounded rectangle.

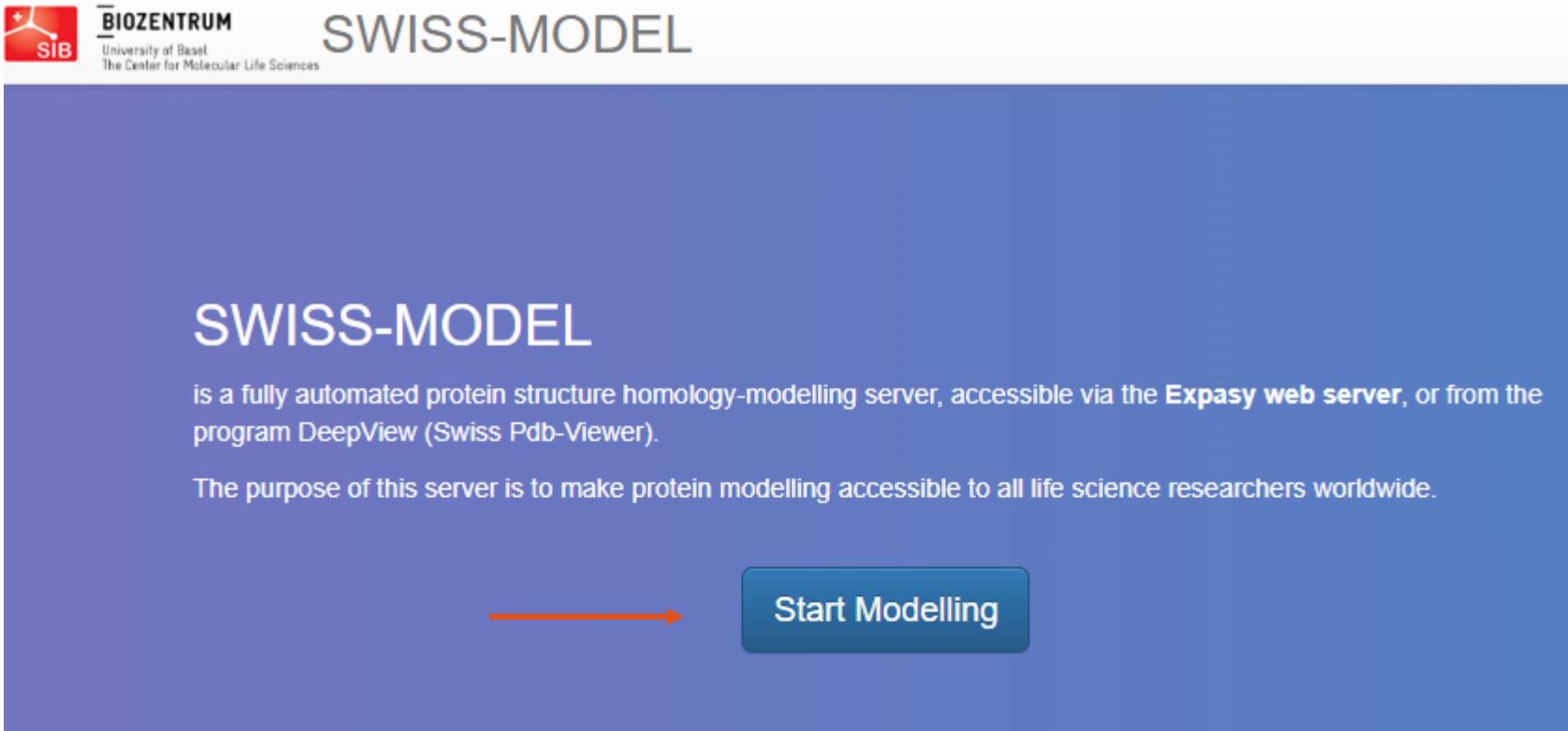
viu

Universidad
Internacional
de Valencia

Modelado por homología

Swiss Model

<https://swissmodel.expasy.org>



The screenshot shows the homepage of the SWISS-MODEL server. At the top left is the SIB logo (a red square with a white stylized 'S') and the BIOZENTRUM logo (a blue square with a white stylized 'B'). To the right of these is the text 'SWISS-MODEL' and 'University of Basel The Center for Molecular Life Sciences'. The main title 'SWISS-MODEL' is centered on a blue background. Below it, a paragraph explains that it is a fully automated protein structure homology-modelling server accessible via the Expasy web server or DeepView. A second paragraph states the purpose is to make protein modelling accessible to all life science researchers worldwide. At the bottom right is a teal button with the text 'Start Modelling'.

Modelado por homología

Swiss Model

Crear un modelo nuevo. Podemos o bien pegar directamente la secuencia FASTA de nuestra proteína (1) o subir un archivo FASTA que la contenga (2). Buscar estructuras molde (3).

The screenshot shows the SWISS-MODEL web interface for starting a new modelling project. The interface is divided into several sections:

- Header:** SWISS-MODEL, BIOZENTRUM, University of Basel, The Center for Molecular Life Sciences.
- Project Title:** Untitled Project (highlighted in red)
- Email:** Ingresar email (highlighted in red)
- Target Sequence(s):** A text input field with placeholder text "Paste your target sequence(s) or UniProtKB AC here". A green button labeled "+ Upload Target Sequence File..." is next to it. A checkbox labeled "Validate" is also present.
- Template Search:** A blue button labeled "Search For Templates" and a blue button labeled "Build Model".

Three orange circles with numbers 1, 2, and 3 are overlaid on the interface to indicate specific steps:

- 1: Points to the "Paste your target sequence(s) or UniProtKB AC here" input field.
- 2: Points to the "+ Upload Target Sequence File..." button.
- 3: Points to the "Search For Templates" button.

Modelado por homología

Swiss Model

Crear un modelo nuevo. Podemos o bien pegar directamente la secuencia FASTA de nuestra proteína (1) o del alineamiento deseado empleando formato FASTA (2) o Clustal (3).

The screenshot shows the SWISS-MODEL interface. On the left, there's a logo for SIB BIOZENTRUM University of Basel, The Center for Molecular Life Sciences. The main title is "SWISS-MODEL". Below it, there's a section titled "Start a New Modelling Project" with a question mark icon. It has a text input field labeled "Paste your target sequence(s) or UniProtKB AC here" (marked with a red circle 1). Below the input field are two buttons: "+ Upload Target Sequence File..." and "Validate". To the right of the input field, there are examples for FASTA and Clustal formats. The FASTA example (marked with a red circle 2) shows two sequences: THN_DENCL and 1crnA. The Clustal example (marked with a red circle 3) shows a multiple sequence alignment between THN_DENCL and 1crnA.

Example for FASTA:

```
>THN_DENCL  
KSCCPPTAACRNQYNICRLPGTPRPVCAALSGCKIISGTGCPPGYRH-  
>1crnA  
TTCCPSIVARSNFNVCRLPGTPEALCATYTGCIIIPGATCPGDYAN-
```

Example for Clustal:

```
CLUSTAL W (1.82) multiple sequence alignment  
THN_DENCL      KSCCPPTAACRNQYNICRLPGTPRPVCAALSGCKIISGTGCPPGYRH- 46  
1crnA          TTCCPSIVARSNFNVCRLPGTPEALCATYTGCIIIPGATCPGDYAN- 46  
. :***   ..* : **: * .. :** :** ***..: **  *
```

Modelado por homología

Swiss Model

Esperar mientras el servidor busca la secuencia molde más apropiada. Puede tardar varios minutos dependiendo de la longitud de la secuencia. Mientras tanto, verá una ventana parecida a la que se muestra aquí.

trpv1 Created: today at 09:00

Summary **Templates** Models Project Data ▾

Template Results

The search for templates matching your target sequence is currently running. Please wait.

...running HHblits against SMTL
...reusing cached query alignment
...predicting residue burial status with ACCpro
...searching PDB profile database with previously built query profile

Aquí se especifica cada paso que tiene lugar en la búsqueda del molde.

If you want to come back later, bookmark this link:

<https://swissmodel.expasy.org/interactive/RR8NvZ/>

The sequence logo visualization shows the search for a template match. The sequence is composed of several colored segments: blue, cyan, green, orange, and yellow. The blue segment spans from approximately position 10 to 40. The cyan segment spans from approximately position 45 to 75. The green segment spans from approximately position 80 to 110. The orange segment spans from approximately position 115 to 145. The yellow segment spans from approximately position 150 to 180. Each segment contains a different set of amino acid residues, representing the consensus sequence at that position. The background is white, and the overall pattern suggests a search space being narrowed down through iterative steps.

Modelado por homología

Swiss Model

Esperar mientras el servidor busca la secuencia molde más apropiada. Puede tardar varios minutos dependiendo de la longitud de la secuencia. Mientras tanto, verá una ventana parecida a la que se muestra aquí.

The search for templates matching your target sequence is currently running. Please wait.

```
...running HHblits against SMTL
...reusing cached query alignment
...predicting residue burial status with ACCpro
...searching PDB profile database with previously built query profile
...running BLAST against SMTL
...running AFDB template search
...searching AFDB sequence database with target sequence
...getting AFDB templates
...extracting distance constraints from 4960 templates
...filtering list of templates
...structurally superpose templates
...predicting oligomeric state conservation
```

Modelado por homología

Swiss Model

Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:

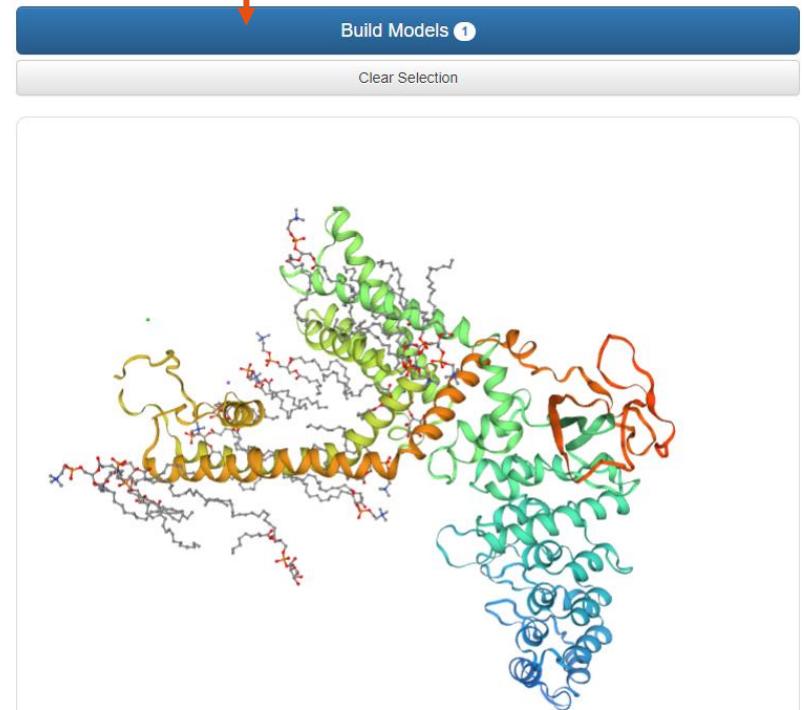
Summary Templates **23** Models Project Data ▾

Template Results

Templates Quaternary Structure Sequence Similarity Alignment More ▾

↓↓ Sort	Coverage	GMQE	QSQE	Identity	Method	Oligo State	Ligands
<input checked="" type="checkbox"/> 7lqy.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in apo state	0.78	0.95	85.35	EM	homo-tetramer ✓	32 x POV [⌚] , 4 x YBG [⌚]	
<input type="checkbox"/> 7lqy.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in apo state	0.78	0.95	89.26	EM	homo-tetramer ✓	32 x POV [⌚] , 4 x YBG [⌚]	
<input type="checkbox"/> 7lp9.1.A Transient receptor potential cation channel subfamily V member 1 Cryo-EM structure of full-length TRPV1 at 4 degrees Celsius	0.76	0.95	86.14	EM, 2.6 Å	homo-tetramer ✓	4 x T7X [⌚] , 8 x LBN [⌚] , 28 x 6OU [⌚] , 4 x YFP [⌚]	
<input type="checkbox"/> 7lpa.1.A Transient receptor potential cation channel subfamily V member 1 Cryo-EM structure of full-length TRPV1 with capsaicin at 4 degrees Celsius	0.73	0.96	86.14	EM, 3.4 Å	homo-tetramer ✓	8 x LBN [⌚] , 12 x 6OU [⌚] , 4 x 4DY [⌚] , 4 x YFP [⌚]	
<input type="checkbox"/> 7rqu.1.B Transient receptor potential cation channel subfamily V member 1 Cryo-EM structure of the full-length TRPV1 with RTx at 4 degrees Celsius, in a closed state, class I	0.75	0.94	86.14	EM	homo-tetramer ✓	4 x 6EU [⌚] , 8 x LBN [⌚] , 20 x 6OU [⌚] , 4 x YFP [⌚]	
<input type="checkbox"/> 7lqz.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in complex with RTx	0.76	0.92	85.35	EM	homo-tetramer ✓	32 x POV [⌚] , 4 x 6EU [⌚]	
<input type="checkbox"/> 7lqz.1.A Osm-9-like TRP channel 1 Structure of squirrel TRPV1 in complex with RTx	0.76	0.92	89.26	EM	homo-tetramer ✓	32 x POV [⌚] , 4 x 6EU [⌚]	

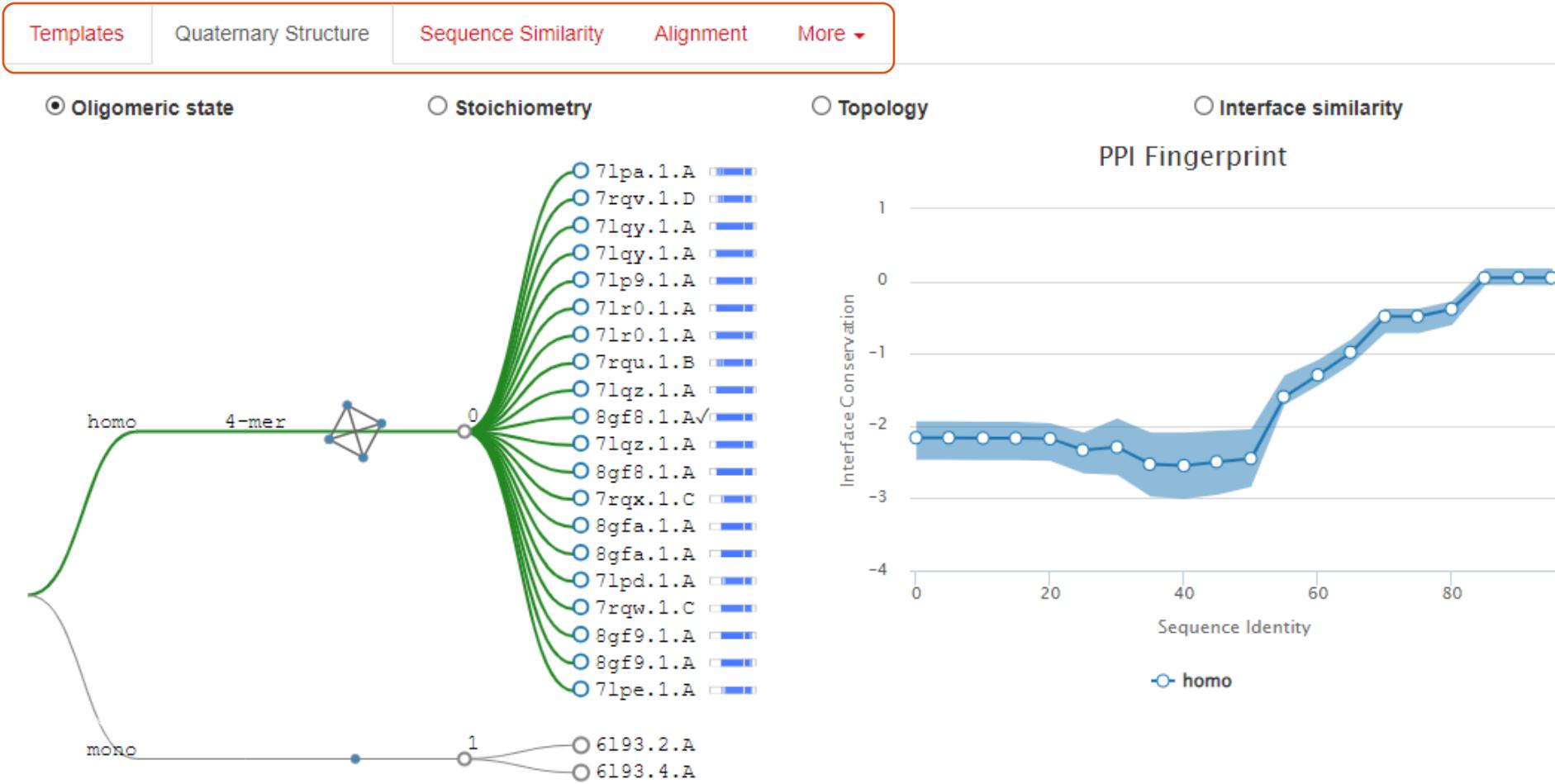
Construir modelo según molde seleccionado



Modelado por homología

Swiss Model

Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:

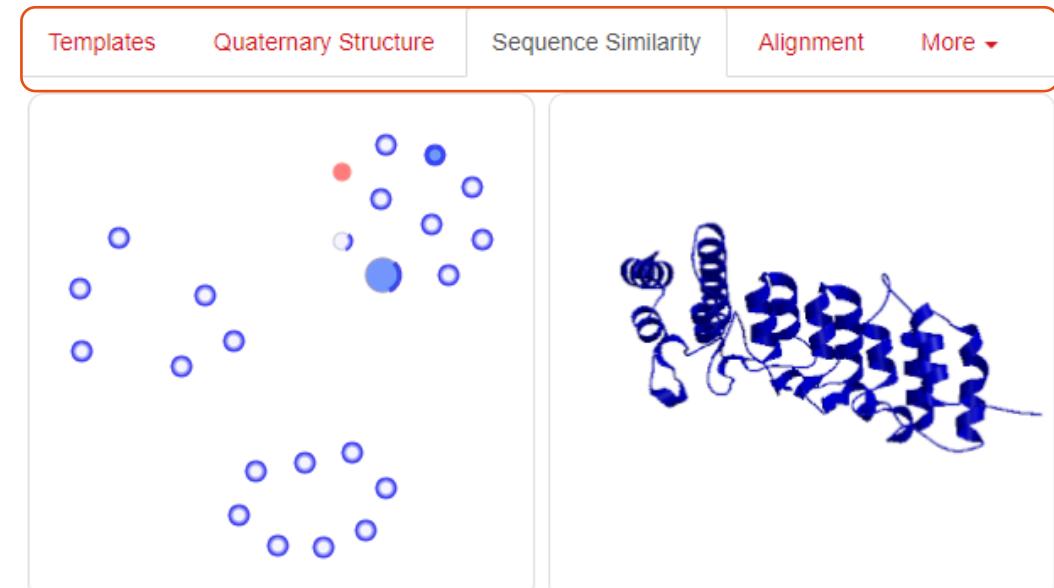


Modelado por homología

Swiss Model

Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:

Templates Quaternary Structure Sequence Similarity Alignment More ▾



Template: 6I93.2.A Transient receptor potential cation channel subfamily V member 1
X-ray structure of the ligand-free human TRPV1 ankyrin repeat domain

Coverage: 100.00

Identity: 100.00

Similarity: 0.61

Ligands: -

Method: X-ray 4.47 Å

Oligo State: monomer

Found By: BLAST

Modelado por homología

Swiss Model

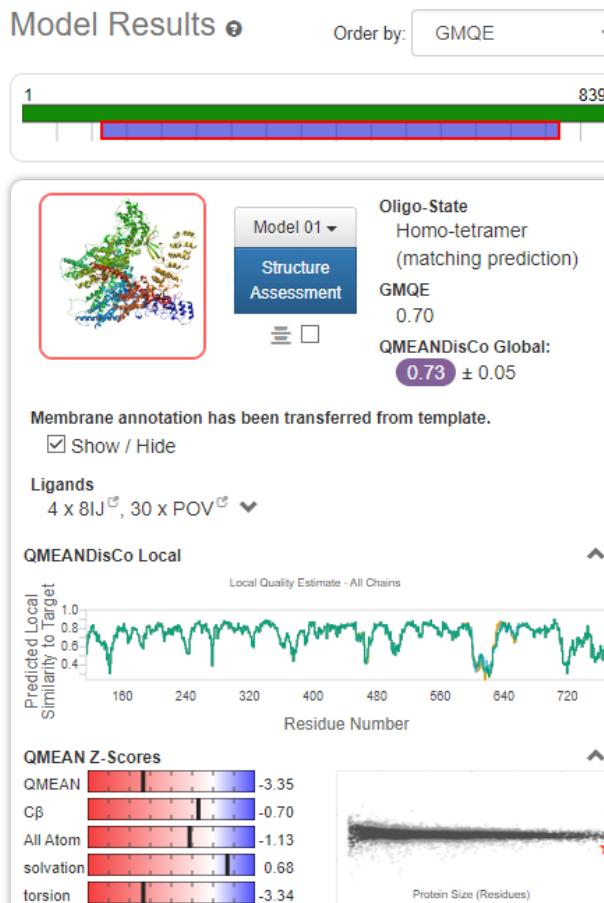
Una vez haya finalizado la búsqueda veremos la siguiente tabla de resultados:

	Templates	Quaternary Structure	Sequence Similarity	Alignment	More ▾
Target	MKKWSSTDLGAAADPLQKDTCPDPLGDPNNSRPPPAKPQLSTAKSRTLFGKDSEEAFTPVDCHHEEGELDSCPCTITVSPVITIQRPGDGPTGARLLSQDSVAAS				
8gf8.1.A	-KKWSSSTDLGAAADPLQKDTCPDPLGDPNNSRPPPAKPQLSTAKSRTLFGKDSEEAFTPVDCHHEEGELDSCPCTITVSPVITIQRPGDGPTGARLLSQDSVAAS				
6193.2.A	-				SVAAS
Target	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLFLQKSKKHLDNEFKDPETGKTCLLKAMLNLDHGQNTTIPILLIEIARQTDSDLKELVNASYTDYYKGQTALHIAI				
8gf8.1.A	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLFLQKSKKHLDNEFKDPETGKTCLLKAMLNLDHGQNTTIPILLIEIARQTDSDLKELVNASYTDYYKGQTALHIAI				
6193.2.A	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLFLQKSKKHLDNEFKDPETGKTCLLKAMLNLDHGQNTTIPILLIEIARQTDSDLKELVNASYTDYYKGQTALHIAI				
Target	ERRNMALVTLLVENGADVQAAAHDFFKKTKGRPGFYFGEPLSLAACTNQLGIVKFLLQNSWQTADISARDSVGNTVLHALVEADNTADNTKFVTSMYNEILM				
8gf8.1.A	ERRNMALVTLLVENGADVQAAAHDFFKKTKGRPGFYFGEPLSLAACTNQLGIVKFLLQNSWQTADISARDSVGNTVLHALVEADNTADNTKFVTSMYNEILM				
6193.2.A	ERRNMALVTLLVENGADVQAAAHDFFKKTKGRPGFYFGEPLSLAACTNQLGIVKFLLQNSWQTADISARDSVGNTVLHALVEADNTADNTKFVTSMYNEILM				
Target	LGAKLHPTLKLEELTNKKGMTPLALAAGTGKIGVLAYILQREIQEPECRHLSRKFTEWAYGPVHSSLYDLS CIDTCEKNSVLEVIAYSSETPNRHDMILLVEPLN				
8gf8.1.A	LGAKLHPTLKLEELTNKKGMTPLALAAGTGKIGVLAYILQREIQEPECRHLSRKFTEWAYGPVHSSLYDLS CIDTCEKNSVLEVIAYSSETPNRHDMILLVEPLN				
6193.2.A	LGAKLHPTLKLEELTNKKGMTPLALAAGTGKIGVLAYILQREIQEPECRH				
Target	RLLQDKWDRFVKRIFYFNFLVYCLYMIIFTMAAYYRPVDGLPPFKMEKTGDYFRVTGEILSVLGGVYFFF RGIQYFLQRRPSMKTLFVDSYSEM LFFLQSLFMLA				
8gf8.1.A	RLLQDKWDRFVKRIFYFNFLVYCLYMIIFTMAAYYRPVDGLPPFKMEKTGDYFRVTGEILSVLGGVYFFF RGIQYFLQRRPSMKTLFVDSYSEM LFFLQSLFMLA				
6193.2.A	-				
Target	TVVLYFSHLKEYVASMVFSLALGWTNMLYYTRGFQQMGIYAVMIEKMLRDLCRMFMVYIVFLFGFSTAVVTLIEDGKNDSLPESTSHRWRGACRPPDSSYNS				
8gf8.1.A	TVVLYFSHLKEYVASMVFSLALGWTNMLYYTRGFQQMGIYAVMIEKMLRDLCRMFMVYIVFLFGFSTAVVTLIEDGKNDSLPESTSHRWRGACRPPDSSYNS				
6193.2.A	-				
Target	LYSTCLELFKFTIGMDLEFTENYDFKAVFIILLAYVILTYIILNLIALMGETVNKIAQESKNIWKLR AITILDTEKSFLKCMRKAFRSGKLLQVG YTPDG				
8gf8.1.A	LYSTCLELFKFTIGMDLEFTENYDFKAVFIILLAYVILTYIILNLIALMGETVNKIAQESKNIWKLR AITILDTEKSFLKCMRKAFRSGKLLQVG YTPDG				
6193.2.A	-				
Target	KDDYRWCFRVDEVNWTWNNTN VGIINEDPGNCEGVKRTLSFSRSLSSRVSGRHWNFALVPLLREASARDQSAQPEEVYLQFSGSLKPEDAEVFKSPAASGEK				
8gf8.1.A	KDDYRWCFRVDEVNWTWNNTN VGIINEDPGNCEGVKRTLSFSRSLSSRVSGRHWNFALVPLLREASARDQSAQPEEVYLQFSGSLKPEDAEVFKSPAASGEK				
6193.2.A	-				

Modelado por homología

Swiss Model

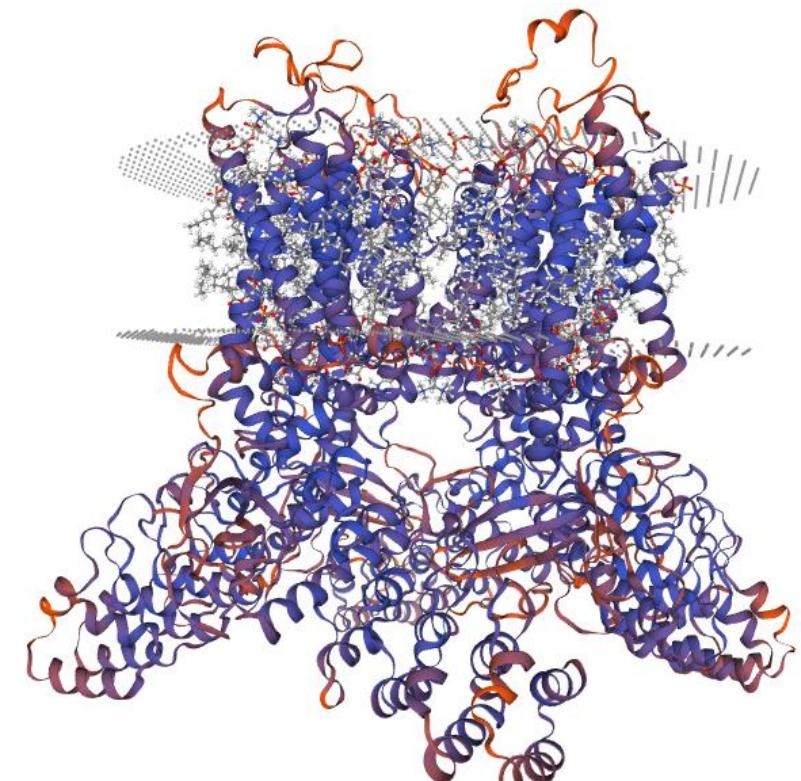
Construcción del modelo según selección anterior.



Template: 8gf8.1.A Transient receptor potential cation channel subfamily V member 1 Seq Identity: 100.00% Coverage: 100.00%

Model-Template Alignment:

Model Chain	Template Chain	Sequence	Length
Model_01:A	8gf8.1.A	MKKWSSTDLGAAADPLQKDTCPDPPLGDGPNSRPPP	35
Model_01:B	8gf8.1.B	MKKWSSTDLGAAADPLQKDTCPDPPLGDGPNSRPPP	35
Model_01:C	8gf8.1.C	MKKWSSTDLGAAADPLQKDTCPDPPLGDGPNSRPPP	35
Model_01:D	8gf8.1.D	MKKWSSTDLGAAADPLQKDTCPDPPLGDGPNSRPPP	35
Model_01:A	8gf8.1.A	-KKWSSTDLGAAADPLQKDTCPDPPLGDGPNSRPPP	37
Model_01:B	8gf8.1.B	-AKPQLSTAKSRTRLFGKGDSEEAFPVDCPHEEGEL	70
Model_01:C	8gf8.1.C	-AKPQLSTAKSRTRLFGKGDSEEAFPVDCPHEEGEL	70
Model_01:D	8gf8.1.D	-AKPQLSTAKSRTRLFGKGDSEEAFPVDCPHEEGEL	70
Model_01:A	8gf8.1.A	-AKPQLSTAKSRTRLFGKGDSEEAFPVDCPHEEGEL	72
Model_01:B	8gf8.1.B	DSCPTITVSPVITIQRPGDGPTGARLLSQDSVAAS	105
Model_01:C	8gf8.1.C	DSCPTITVSPVITIQRPGDGPTGARLLSQDSVAAS	105
Model_01:D	8gf8.1.D	DSCPTITVSPVITIQRPGDGPTGARLLSQDSVAAS	105
Model_01:A	8gf8.1.A	DSCPTITVSPVITIQRPGDGPTGARLLSQDSVAAS	107
Model_01:B	8gf8.1.B	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLLFLQKS	140
Model_01:C	8gf8.1.C	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLLFLQKS	140
Model_01:D	8gf8.1.D	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLLFLQKS	140
Model_01:A	8gf8.1.A	TEKTLRLYDRRSIFEAVAQNNCQDLESLLLLFLQKS	142
Model_01:B	8gf8.1.B	KKHLTDNEFKDPETGKTCLLKAMLNLDGQNTTIP	175
Model_01:C	8gf8.1.C	KKHLTDNEFKDPETGKTCLLKAMLNLDGQNTTIP	175
Model_01:D	8gf8.1.D	KKHLTDNEFKDPETGKTCLLKAMLNLDGQNTTIP	175
Model_01:A	8gf8.1.A	KKHLTDNEFKDPETGKTCLLKAMLNLDGQNTTIP	177
Model_01:B	8gf8.1.B	LLLEIARQTDSLKELVNASYTDSYYKGQTALHIAI	210
Model_01:C	8gf8.1.C	LLLEIARQTDSLKELVNASYTDSYYKGQTALHIAI	210
Model_01:D	8gf8.1.D	LLLEIARQTDSLKELVNASYTDSYYKGQTALHIAI	210
Model_01:A	8gf8.1.A	LLLEIARQTDSLKELVNASYTDSYYKGQTALHIAI	212



Modelado por homología

Swiss Model

Error en proporcionar un modelo fiable.





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