



Central European Institute of Technology  
BRNO | CZECH REPUBLIC

# Biomacromolecular structure analysis - channels

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EUROPEAN UNION  
EUROPEAN REGIONAL DEVELOPMENT FUND  
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Development for Innovation**



## MOLEonline: Web application for detection of channels and pores and calculation of their geometrical and physico-chemical properties

### New features:

- Automatic detection of transmembrane pores
- Visualization of properties on the channel's profile
- Interconnection with other bioinformatics tools (PDBe, CSA, ChannelsDB, OPM, UniProt) and data transfer from them
- Integration of LiteMol suite

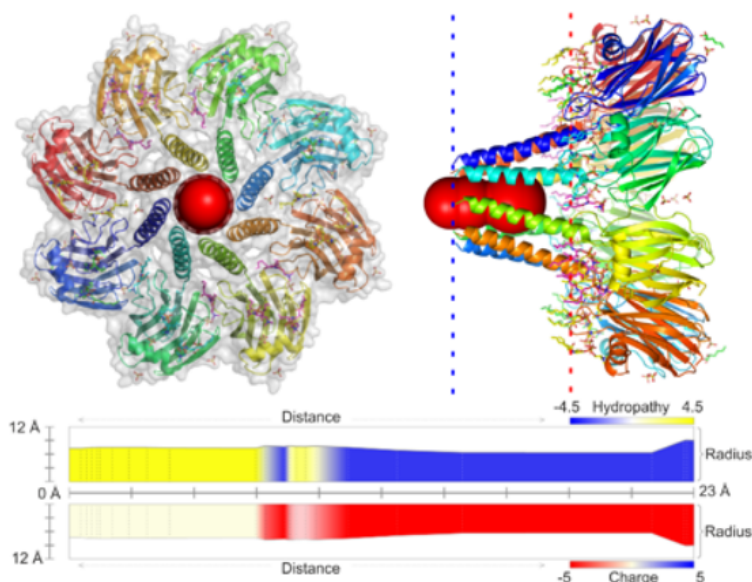
• Pravda L., Sehnal D., Toušek D., Navrátilová V., Bazgier V., Berka K., ... & **Koča J.**, Otyepka M. (2018). *MOLEonline: a web-based tool for analyzing channels, tunnels and pores (2018 update)*. **Nucleic acids research**.

## MOLEonline

[Home](#)[Online](#)[Documentation](#)[About](#)

**MOLEonline** web interface provides a direct access to MOLE functionality and enables on-line and easy-to-use interactive channel analysis.

**MOLE 2.5** is an universal toolkit for **rapid and fully automated location and characterization of channels, tunnels and pores** in (bio)macromolecular structures, e.g., proteins, RNA, DNA and biomacromolecular assemblies.



### MOLEonline features

- Quickest channel calculation on the market
- Automatic transmembrane pore identification
- Layered channel profile - geometry, length and radius
- List of residues lining channels (distinguishing sidechain/mainchain contact with the channel)
- Layered or channel-wise physico-chemical properties (several types of channel radius, length, charge, polarity, hydropathy, hydrophobicity, mutability, etc.)

### Quick start

PDBID File Last session

PDB ID:  ?

Assembly ID (optional):  ?

Use biological unit:  ?

[Next](#)

### News

#### Attention 8. 6. 2019

Update to Chrome 75 disables WebGL functionalities important for MOLEonline LiteMol visualization. We are working on fix on this issue. Meanwhile use other browsers for accessing MOLEonline.

#### Server room maintenance 17. 12. 2018

We would like to announce that MOLEonline will not be available on Monday (December 17th) due to web server room maintenance. Sorry for the inconvenience.

#### MOLEonline update 2018 was published 1. 5. 2018


Our paper, which describes the new features of MOLEonline, is accepted for publication in [Web issue of Nucleic Acids Research](#).

#### New features and updates 2. 4. 2018

New features in MOLEonline:

- new Help button will allow to send us your troubled session so we can help you more thoroughly,
- multiple layers can be selected/deselected to show average properties

1tqn ChannelsDB Download Help



Protein Sequence ↑

Chain A H S H G L F K K L G I P G P T P L P F L G N I L S Y H K G F C M F D M E C H K K Y G K V W G F Y D G Q Q P V L A I T D P D M I K T V L V K E C Y S V F T N R R P F G P V G

28 48 68 88 108

128 148 168 188

Profile Channels properties

Layer Lining residues Phys. Chem. Properties

**Residue**

Hover over channel(2D) for details...

**Property Value**

Hover over channel(2D) for details...

**Selection**

Click on atom residue or channel

**Channels**

There are no channels available...

**Origins**

Computed

CSA Origins

**Cavities**

+ Surface (1)

Submission settings Submissions

**Channels** Switch to Pore mode

▼ **Active Atoms/Residues**

Ignore HETATMs ✓ On

► **Advanced options**

► **Cavity Parameters**

► **Channel Parameters**

▼ **Selection**

Starting Point	Current Selection	
	✓	Add
Selected Points		
No starting points		
End Point	Current Selection	
	✓	Add

Submit Kill Delete Clear

**Quick help**

**How to start? Try this:**

- For automatic start just press Submit button
- Or select specific **Start or End points**
  - by **XYZ** coordinate or **residue** selection in 3D or from sequence,
  - or try to use the Catalytic Active Sites from **CSA** or **cofactors** (Panel **Selection**),
  - or use facet selection on **Surface** in 3D viewer using Ctrl+left mouse click,
  - Or in the structure from precomputed **Origin** points, and press Submit button.

1tqn ChannelsDB Download Help



Protein Sequence ↑

Chain A 28 H S H G L F K K L G I P G P T P L P F L G N I L S Y H K G F C M F D M E C H K K Y G K V W G F Y D G Q Q P V L A I T D P D M I K T V L V K E C Y S V F T N R R P F G P V G  
 48 68 88 108  
 128 148 168 188

Profile Channels properties

Layer Lining residues Phys. Chem. Properties

**Residue**

Hover over channel(2D) for details...

Property	Value
Hover over channel(2D) for details...	

**Selection**

Click on atom residue or channel

**Channels**

There are no channels available...

**Origins**

Computed  
 CSA Origins

**Cavities**

+ Surface (1)

Submission settings Submissions

**Channels** [Switch to Pore mode](#)

▼ **Active Atoms/Residues**

Ignore HETATMs  On

► **Advanced options**

► **Cavity Parameters**

► **Channel Parameters**

▼ **Selection**

Starting Point	Current Selection	
	<input checked="" type="checkbox"/>	Add
Selected Points		
No starting points		
End Point	Current Selection	
	<input checked="" type="checkbox"/>	Add

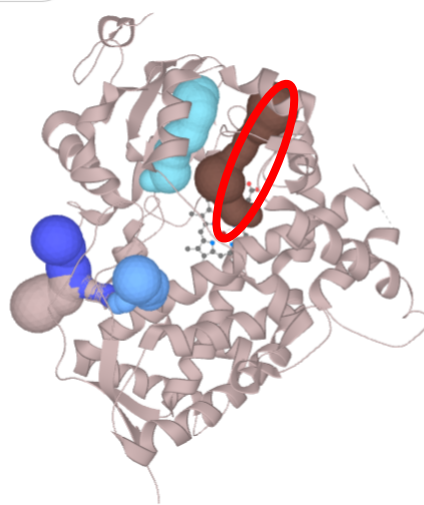
**Submit** **Delete** **Clear**

## Quick help

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1tqn ChannelsDB Download Help



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Chain A 28 H S H G L F K K L G I P G P T L P L F L G N I L S Y H K G F C M F D M E C H K K Y G K V W G F Y D G Q Q P V L A I T D P D M I K T V L V K E C Y S V F T N R R P F G P V G 108  
 128 148 168 188

Channel profile Channels properties

Layer Lining residues Phys. Chem. Properties

**Residue**

Hover over channel(2D) for details...

**Property** Value

Hover over channel(2D) for details...

Submit Kill Delete Clear 1

**Selection**

Click on atom residue or channel

**Channels**

+ Tunnels (27)

**Origins**

Computed  
 CSA Origins

**Cavities**

+ Surface (1)

Submission settings Submissions

**Channels** Switch to Pore mode

▼ **Active Atoms/Residues**

Ignore HETATMs ✓ On

▶ **Advanced options**

▶ **Cavity Parameters**

▶ **Channel Parameters**

▼ **Selection**

Starting Point	Current Selection	
	✓	Add
Selected Points		
No starting points		
End Point	Current Selection	
	✓	Add


Quick help

**To see channel results:**

- You can:
  - Pick one of available channels either in **list of channels** or in **3D view** window to see **Channel profile** with mapped physicochemical properties and residues associated with tunnel **layers** or **lining residues** of selected tunnel.
  - See summary of properties of all available channels upon switch to **Channels properties** tab in bottom-left part of screen.
  - Try to compare your data with channels from [ChannelsDB](#) - click on **#ChDB** submission located on **Submission** tab in the bottom right side of the screen.

For more information see [documentation page](#)

1tqn ChannelsDB Download Help

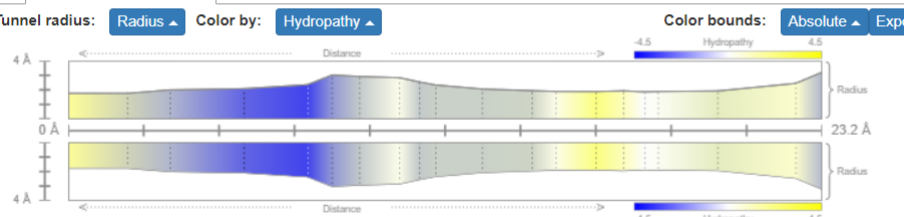


Protein Sequence ↑

Chain A 28 H S H G L F K K L G I P G P T L P L F L G N I L S Y H K G F C M F D M E C H K K Y G K V W G F Y D G Q Q P V L A I T D P D M I K T V L V K E C Y S V F T N R R P F G P V G 108  
 128 F M G A L G L A E D F E W Q L R E L L C R T E T S C K I K E M P L L I O X C R V L Y N L D R A E T C K D V T L K O V E C A Y M D N L T C T F E C V N L D C L N 168 188

Channel profile (T5C1) Channels properties

Tunnel radius: Radius Color by: Hydropathy Color bounds: Absolute Export



Tunnel radius: Radius Color by: Hydropathy

Layer Lining residues Phys. Chem. Properties

Residue	Property	Value
Hover over channel(2D) for details...		
Hover over channel(2D) for details...		

**Selection**

Tunnel (T5C1), Length: 23.2 Å

**Channels**

+ Tunnels (27)

**Origins**

Computed  
 CSA Origins

**Cavities**

+ Surface (1)

Submission settings Submissions

**Channels** [Switch to Pore mode](#)

▼ **Active Atoms/Residues**

Ignore HETATMs  On

► **Advanced options**

► **Cavity Parameters**

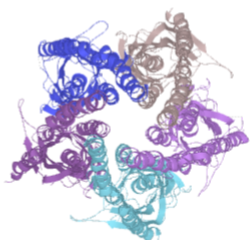
► **Channel Parameters**

▼ **Selection**

Starting Point	Current Selection	
	<input checked="" type="checkbox"/>	Add
Selected Points		
No starting points		
End Point	Current Selection	
	<input checked="" type="checkbox"/>	Add

Submit Kill Delete Clear

< 1 >



Protein Sequence

Chain A	1	21	41	61	81
	SEHETRLVANLLENYNKVI	RPVEHHTHFVDITVGLQL	QLINVDEVNQIVETNVRL	RQQWIDVRLRWNPADYGG	IKKIRLPSDDV
	WLPDLVLYNNADGDFAI	VHMTKLLLDYTGKIMWT	PPAIFKSYCEIIVTHFP	FDQQNCTMKLGIWTDG	TKVSI SPESDRPDLSTF

Profile Channels properties

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  - Or in the structure from precomputed **Origin** points, and press Submit button.



**Selection**

Click on atom residue or channel

**Channels**

There are no channels available...

**Origins**

Computed

**Cavities**

+ Surface (1)

+ Cavities (6)

Submission settings Submissions

**Channels** [Switch to Pore mode](#)

▼ **Active Atoms/Residues**

Ignore HETATMs  On

▶ **Advanced options**

▶ **Cavity Parameters**

▶ **Channel Parameters**

▼ **Selection**

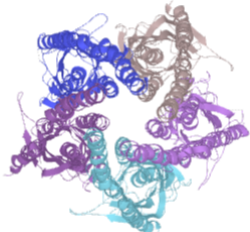
Starting Point	Current Selection	
	<input checked="" type="checkbox"/>	Add
Selected Points		
No starting points		
End Point	Current Selection	
	<input checked="" type="checkbox"/>	Add

Submit Kill Delete Clear



# MOLEonline

2bg9 ChannelsDB Download Help



Selection  
Click on atom residue or channel

Channels  
There are no channels available...

Origins  
 Computed

Cavities  
+ Surface (1)  
+ Cavities (6)

Submission settings Submissions

Pores [Switch to Channels mode](#)

Beta Structure	x	Off
Membrane Region	x	Off
Specific Chains	A, B, ...	
Probe Radius	<input type="range"/>	13
Interior Treshold	<input type="range"/>	0.8

Protein Sequence ↑

Chain A 1 SEHETRLVANLLENYNKVI 21 41 61 81  
101 121 141 161  
WLPDLVLYNNADGDFAI 101 121 141 161  
VHMTKLLLDYTGKIMWTPPAIFKSYCEIIVTHFPFDQQNCTMKGIWTDGTVKVSISPESDRPDLSTF

Profile Channels properties

Layer Lining residues Phys. Chem. Properties

Residue  
Hover over channel(2D) for details...

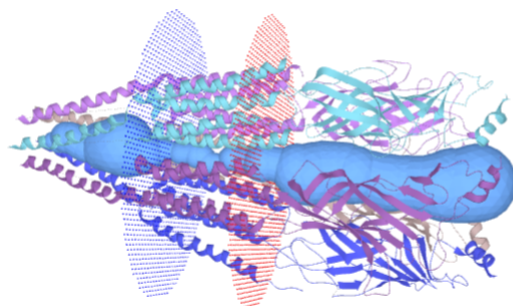
Property Value  
Hover over channel(2D) for details...

Submit Kill Delete Clear

Quick help

How to start? Try this:

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Protein Sequence ↑

Chain A 1 SEHETRLVANLLENYNKVI 21 41 IRPVEHHTHFVDITVGLQLIQLINVDEVNQIVETNVRRLRQQWIDVRLRWNPADYGGIKKIRLPSDDV 81  
 WLPDLVLYNNADGDFAI 101 121 VHMTKLLLDYTGKIMWTPPAIFKSYCEIIVTHFPDQQNCTMKLGIWYDGTKVISIPESDRPDLSTF 141 161

Channel profile Channels properties

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For more information see [documentation page](#).



**Selection** ✖

*Click on atom residue or channel*

**Channels**

+ Paths (1)

**Origins**

Computed

**Cavities**

+ Surface (1)

+ Cavities (1)

Submission settings Submissions ↑

**Pores** Switch to Channels mode

Beta Structure	x Off
Membrane Region	x Off
Specific Chains	A, B, ...
Probe Radius	13
Interior Treshold	0.8

Layer Lining residues Phys. Chem. Properties ↑

**Residue**

Hover over channel(2D) for details...

Property	Value
Hover over channel(2D) for details...	

Submit Kill Delete Clear

< 1 >