

bi-1. PyMOL のインストール と基本機能 (Windows 上)

(バイオインフォマティクスとデータベース)

<https://www.kkaneko.jp/cc/bi/index.html>

金子邦彦



アウトライン



- PyMOL のインストール
- PDB ファイルのダウンロード (RCSB PDB)

- タンパク質構造

PDB ファイルを開く

- リボン図の表示

Hide(H), everything, Show(S), cartoon

The screenshot shows the RCSB PDB website's search results page. The search query is "Advanced Search Query Builder". Two results are displayed:

- 6M2N**: SARS-CoV-2 3CL protease (3CL pro) in complex with a novel inhibitor. Released 2020-04-15. Method: X-RAY DIFFRACTION 2.198 Å. Organism: Severe acute respiratory syndrome coronavirus 2. Macromolecule: SARS-CoV-2 3CL protease (protein). Unique Ligands: 2WL.
- 2Q6G**: Crystal structure of SARS-CoV main protease H41A mutant in complex with an N-terminal substrate. Released 2008-10-12. Method: X-RAY DIFFRACTION 2.5 Å. Organism: SARS coronavirus BJ01. Macromolecule: Polypeptide chain (protein).

The screenshot shows the PyMOL software interface. The title bar reads "PyMOL". The main window displays the 6M2N structure in a green cartoon representation. The command line at the bottom shows the following commands:

```
all R S H L O  
6m2n R S H L O  
Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
R Key Rotate Move Mov2 Slab  
Shift +Box +Box Move2 Slab  
Ctrl Move PRt Pk1 MuS2  
Ctrl Sel0 Drag Clip Move  
SingleClick +/- Cent Menu  
DoubleClick Menu PRt  
Selecting Residues  
State 1/1
```

The screenshot shows the PyMOL software interface with a different view of the 6M2N structure. The title bar reads "PyMOL". The main window displays the 6M2N structure in a green cartoon representation. The command line at the bottom shows the following commands:

```
all R S H L O  
6m2n R S H L O  
Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
R Key Rotate Move Mov2 Slab  
Shift +Box +Box Move2 Slab  
Ctrl Move PRt Pk1 MuS2  
Ctrl Sel0 Drag Clip Move  
SingleClick +/- Cent Menu  
DoubleClick Menu PRt  
Selecting Residues  
State 2/1
```

URL: <https://www.rcsb.org/>

「Coronavirus Proteases sars-cov-2」での検索結果例

RCSB PDB Deposit Search Visualize Analyze Download Learn More

MyPDB

Advanced Search Query Builder

Refinements

Clear All



SCIENTIFIC NAME OF SOURCE ORGANISM

Clear

- Homo sapiens (49498)
- Mus musculus (7087)
- Escherichia coli (6122)
- synthetic construct (5116)
- Escherichia coli K-12 (3559)
- Rattus norvegicus (3215)
- Bos taurus (3049)
- Saccharomyces cerevisiae (2811)
- Saccharomyces cerevisiae S288C (1921)
- Gallus gallus (1848)

More...

TAXONOMY

Clear

- Eukaryota (91632)
- Bacteria (59338)
- Riboviria (8335)
- Archaea (5233)
- artificial sequences (5151)
- Duplodnaviria (2463)
- Varidnaviria (551)

Summary Gallery Compact -- Tabular Report --

Release Date: Newest to Oldest

Download Selected Files

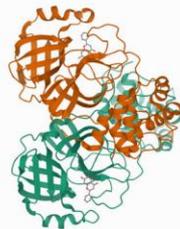
Select All

Displaying 1 to 25 of 169963 Structures

Page 1 of 6799

Previous Next

Display 25 per page



3D View

6M2N

Download File View File

SARS-CoV-2 3CL protease (3CL pro) in complex with a novel inhibitor

Su, H.X., Zhao, W.F., Li, M.J., Xie, H., Xu, Y.C.

To be published

Released 2020-04-15

Method X-RAY DIFFRACTION 2.198 Å

Organisms Severe acute respiratory syndrome coronavirus 2

Macromolecule SARS-CoV-2 3CL protease (protein)

Unique Ligands 3WL



3D View

2Q6G

Download File View File

Crystal structure of SARS-CoV main protease H41A mutant in complex with an N-terminal substrate

Xue, X.Y., Yang, H.T., Xue, F., Bartlam, M., Rao, Z.H.

(2008) J Virol 82: 2515-2527

Released 2008-02-12

Method X-RAY DIFFRACTION 2.5 Å

Organisms SARS coronavirus BJ01

Macromolecule Polypeptide chain (protein)

タンパク質構造の表示 (PyMOL)



PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

Detected GLSL version 4.60.
OpenGL graphics engine:
GL_VENDOR: NVIDIA Corporation
GL_RENDERER: GeForce GTX 970/PCIe/SSE2
GL_VERSION: 4.6.0 NVIDIA 451.67
Detected 8 CPU cores. Enabled multithreaded rendering.

TITLE SARS-CoV-2 3CL protease (3CL pro) in complex with a novel inhibitor

PyMOL>

Reset Zoom Orient Draw/Ray ▾
Unpick Deselect Rock Get View
< < Stop Play > >| MClear
Builder Properties Rebuild

all	A	S	H	L	C
6m2n 1/1	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 Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1

PyMOL>_

◀ ◁ ▢ ▷ ▶ ▶ S ▾ F

リボン図の表示 (PyMOL)



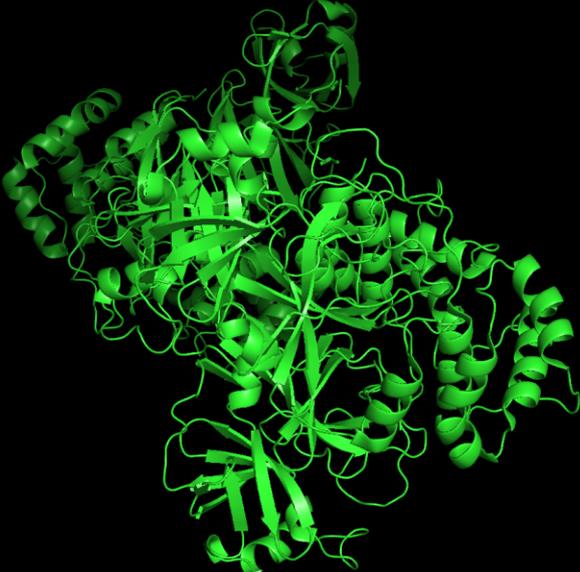
PyMOL

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

GL_VENDOR: NVIDIA Corporation
GL_RENDERER: GeForce GTX 970/PCIe/SSE2
GL_VERSION: 4.6.0 NVIDIA 451.67
Detected 8 CPU cores. Enabled multithreaded rendering.

TITLE SARS-CoV-2 3CL protease (3CL pro) in complex with a novel inhibitor
ExecutiveLoad-Detail: Detected mmCIF
CmdLoad: "D:/Downloads/6m2n.cif/6m2n.cif" loaded as "6m2n".

PyMOL>



all	A	S	H	L	C
6m2n 1/1	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 Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1

PyMOL>_

◀ ◁ ▢ ▷ ▶ ▶ S ▼ F

PyMOL のインストール



1. Python のバージョンを調べる

(あるいは Python をインストールする)

2. Pymol-open-source のダウンロード

- 「Python Extension Packages for Windows - Christoph Gohlke」より、非公式の Windows 版をダウンロード
- ダウンロードするファイルは 2つ.

3. 確認のため「pymol」を実行