

# 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 "SARS-CoV-2 3CL protease (3CL pro) in complex with a novel inhibitor". The results list two structures: 6M2N and 2Q6G. The 6M2N entry is highlighted, showing its title, release date (2020-04-15), method (X-RAY DIFFRACTION 2.198 Å), and organism (Severe acute respiratory syndrome coronavirus 2). The 2Q6G entry is also visible, showing its title, release date (2020-02-12), method (X-RAY DIFFRACTION 2.5 Å), and organism (SARS coronavirus BJ01).

The screenshot shows the PyMOL software interface. The title bar reads "PyMOL". The main window displays the protein structure 6M2N in a green cartoon representation. The command line at the bottom shows "PyMOL>". The status bar at the bottom indicates "State 1/1".

The screenshot shows the PyMOL software interface. The title bar reads "PyMOL". The main window displays the protein structure 6M2N in a green cartoon representation. The command line at the bottom shows "PyMOL>". The status bar at the bottom indicates "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

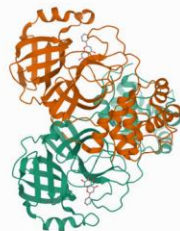
Select All

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

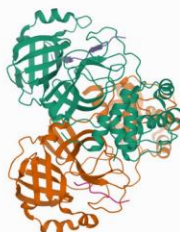
Released 2020-04-15

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>

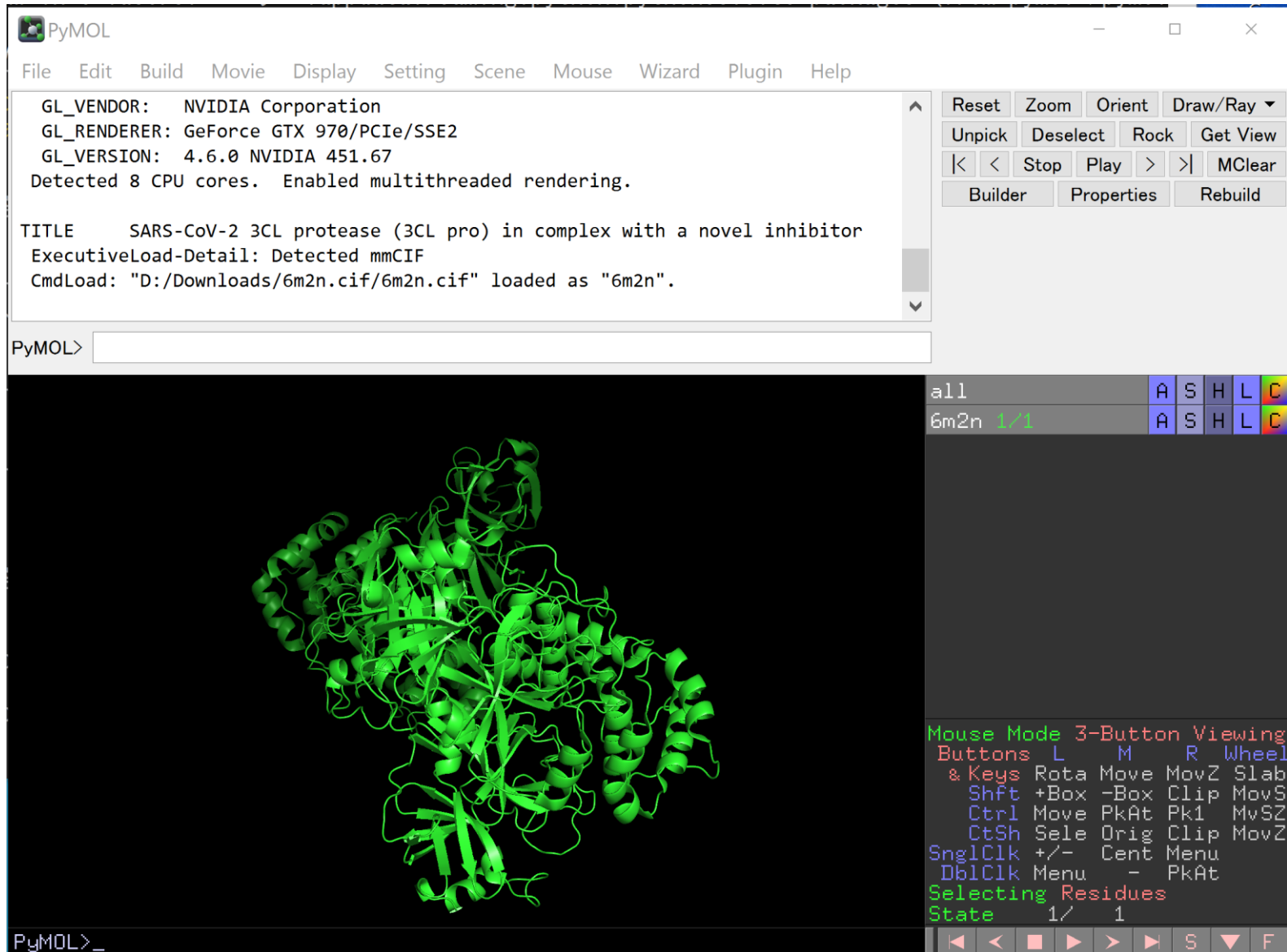
Reset Zoom Orient Draw/Ray  
Unpick Deselect Rock Get View  
< < Stop Play > > MClear  
Builder Properties Rebuild

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>\_

# リボン図の表示 (PyMOL)



The screenshot displays the PyMOL molecular visualization software. The main window shows a 3D ribbon representation of a protein structure in green. The interface includes a menu bar (File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, Help), a status bar at the top with system information (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.), a title bar (TITLE SARS-CoV-2 3CL protease (3CL pro) in complex with a novel inhibitor), and a command line (PyMOL>). A right-hand panel contains various controls (Reset, Zoom, Orient, Draw/Ray, Unpick, Deselect, Rock, Get View, Stop, Play, MClear, Builder, Properties, Rebuild) and a table of object selection options:

Object	A	S	H	L	C
all	■	■	■	■	■
6m2n 1/1	■	■	■	■	■

Below the table, the mouse mode is set to 3-Button Viewing, and the state is 1/1. The bottom status bar shows the PyMOL prompt and navigation icons.

# 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