

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 interface. The search results for PDB entry 6M2N are displayed, including the title "SARS-CoV-2 3CL protease (3CL pro) in complex with a novel inhibitor" and the authors "Sui, H.X., Zhao, W.F., Li, M.J., Xia, H., Xu, Y.C.". The release date is 2020-04-15. The method used is X-RAY DIFFRACTION 2.198 Å. The organisms are "Severe acute respiratory syndrome coronavirus 2" and "SARS-CoV-2 3CL protease (protein)". The macromolecule is "SARS-CoV-2 3CL protease (protein)" and the unique ligands are "2WL".

The screenshot shows the PyMOL software interface. The title bar reads "PyMOL". The main window displays the 3D structure of the SARS-CoV-2 3CL protease in complex with a novel inhibitor, rendered in a green cartoon style. 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 3D structure of the SARS-CoV-2 3CL protease in complex with a novel inhibitor, rendered in a green cartoon style. 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

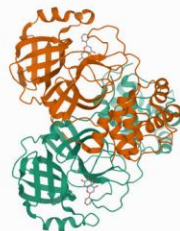
Previous

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

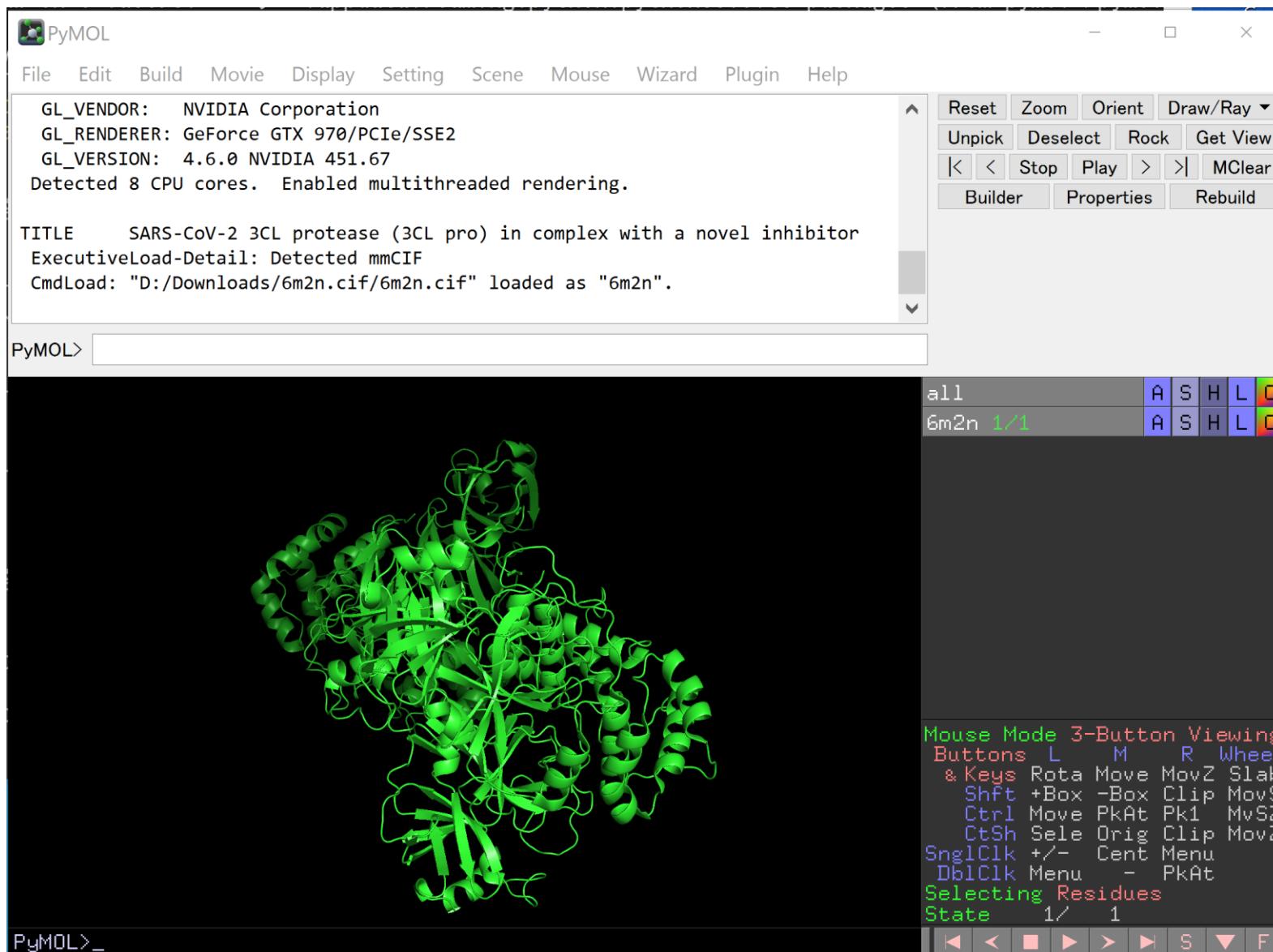
all	A	S	H	L	C
6m2n 1/1	A	S	H	L	C

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>_

◀ ◁ ◻ ▷ ▶ ▶ S ▼ F

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 legend for the protein chain (all, 6m2n 1/1) with color-coded buttons (A, S, H, L, C). A bottom-right panel shows mouse controls (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) and navigation buttons.

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