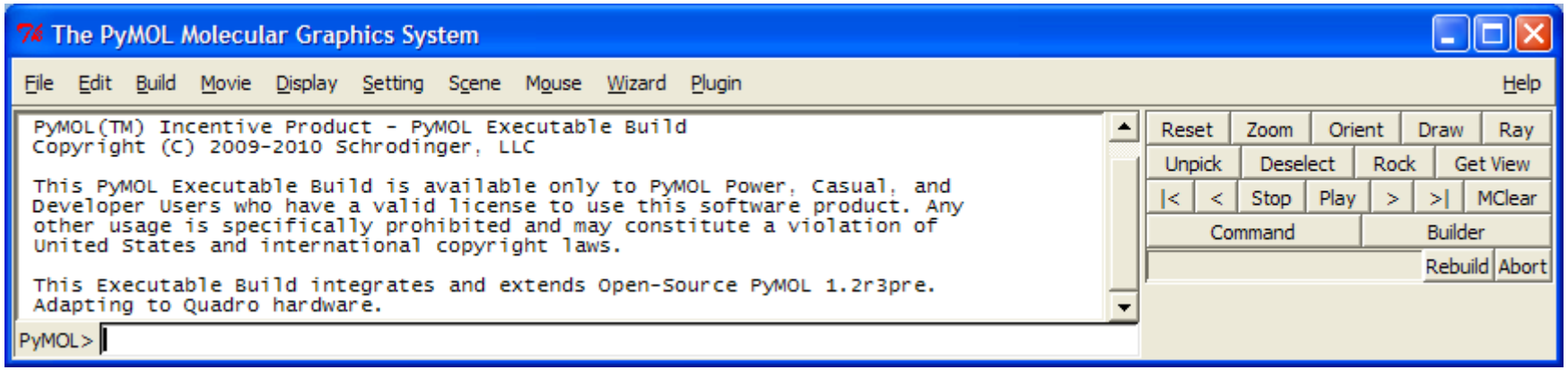
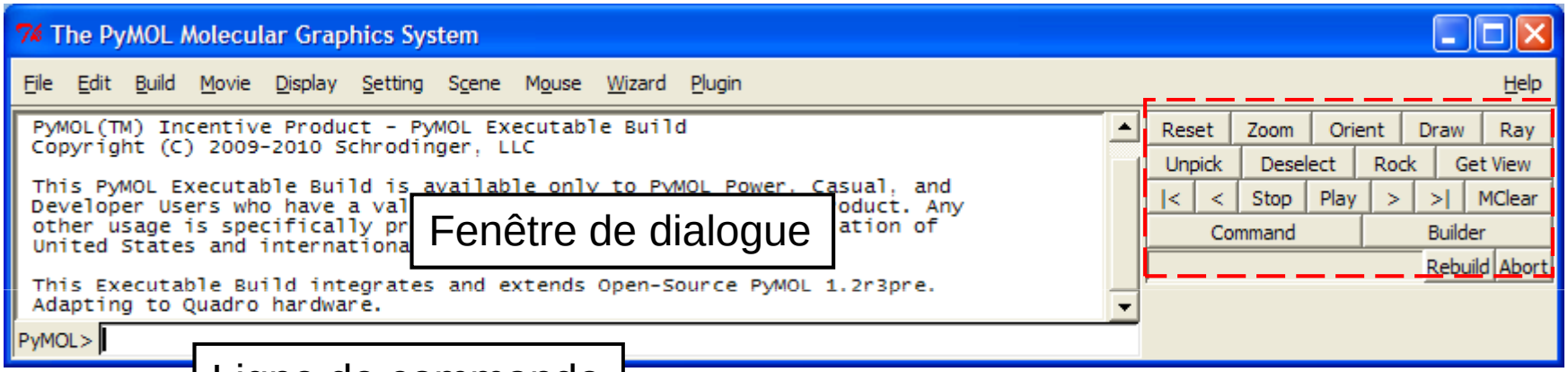
RÉCIPROCS

Pymol



La fenêtre de contrôle
Elle est indépendante

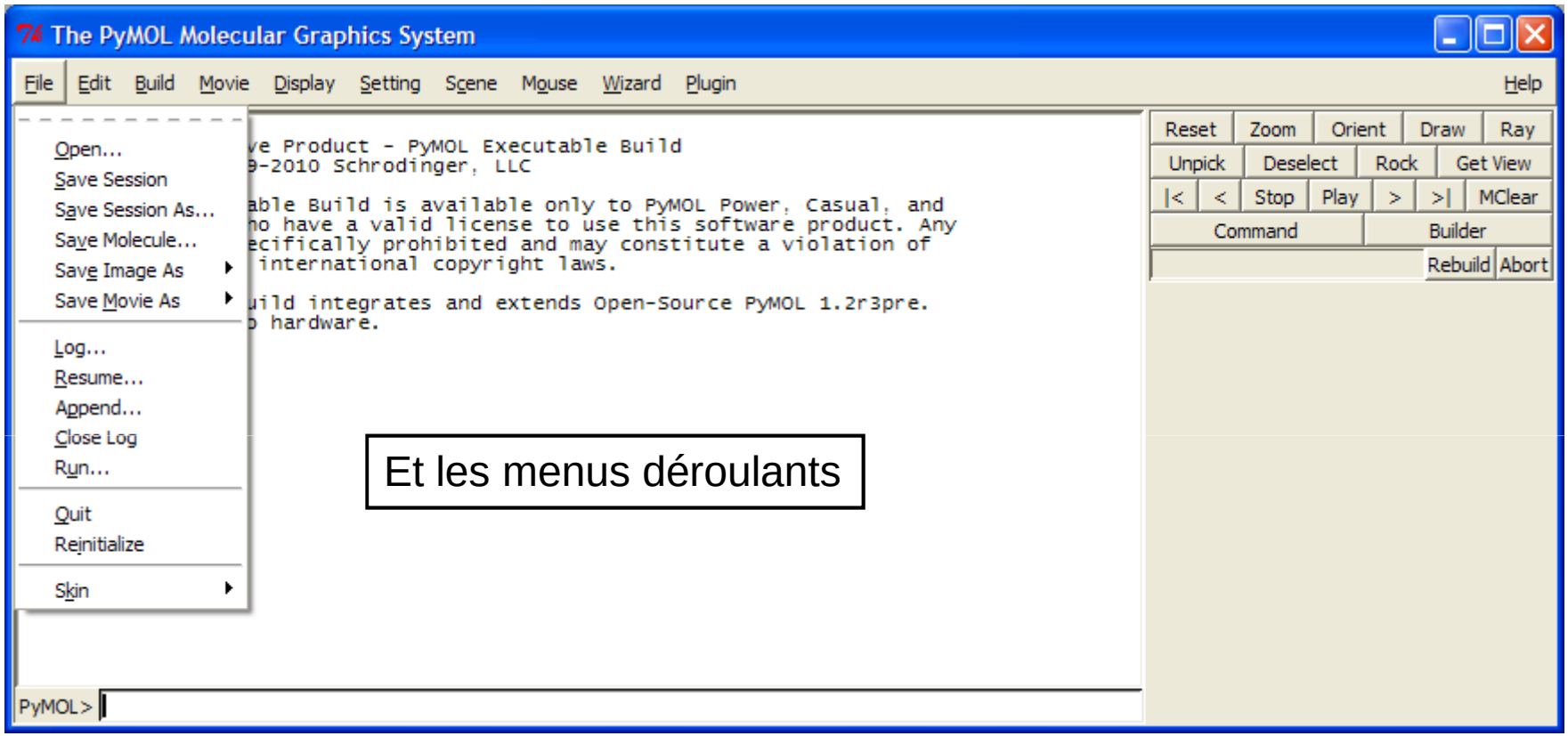


Fenêtre de dialogue

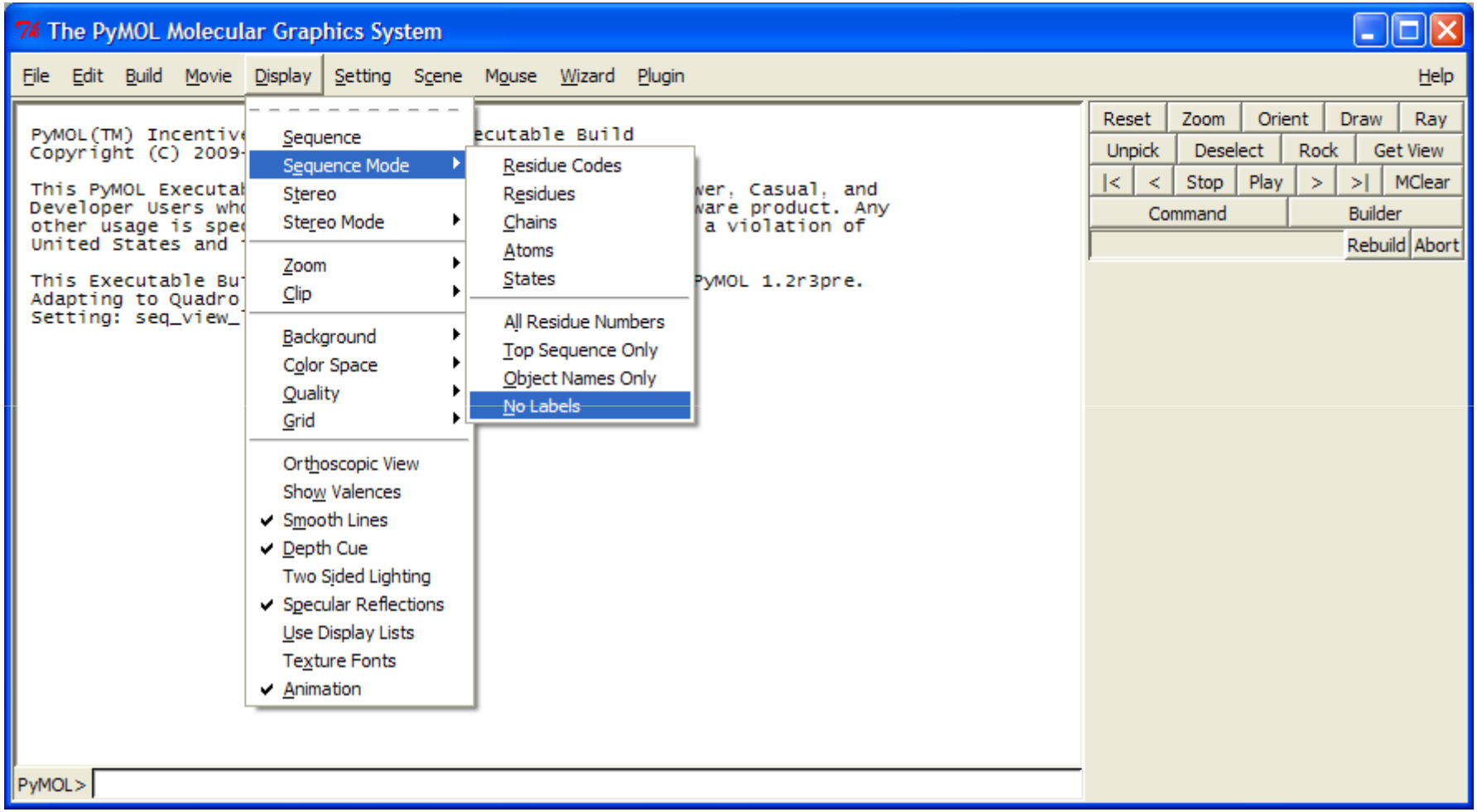
Ligne de commande

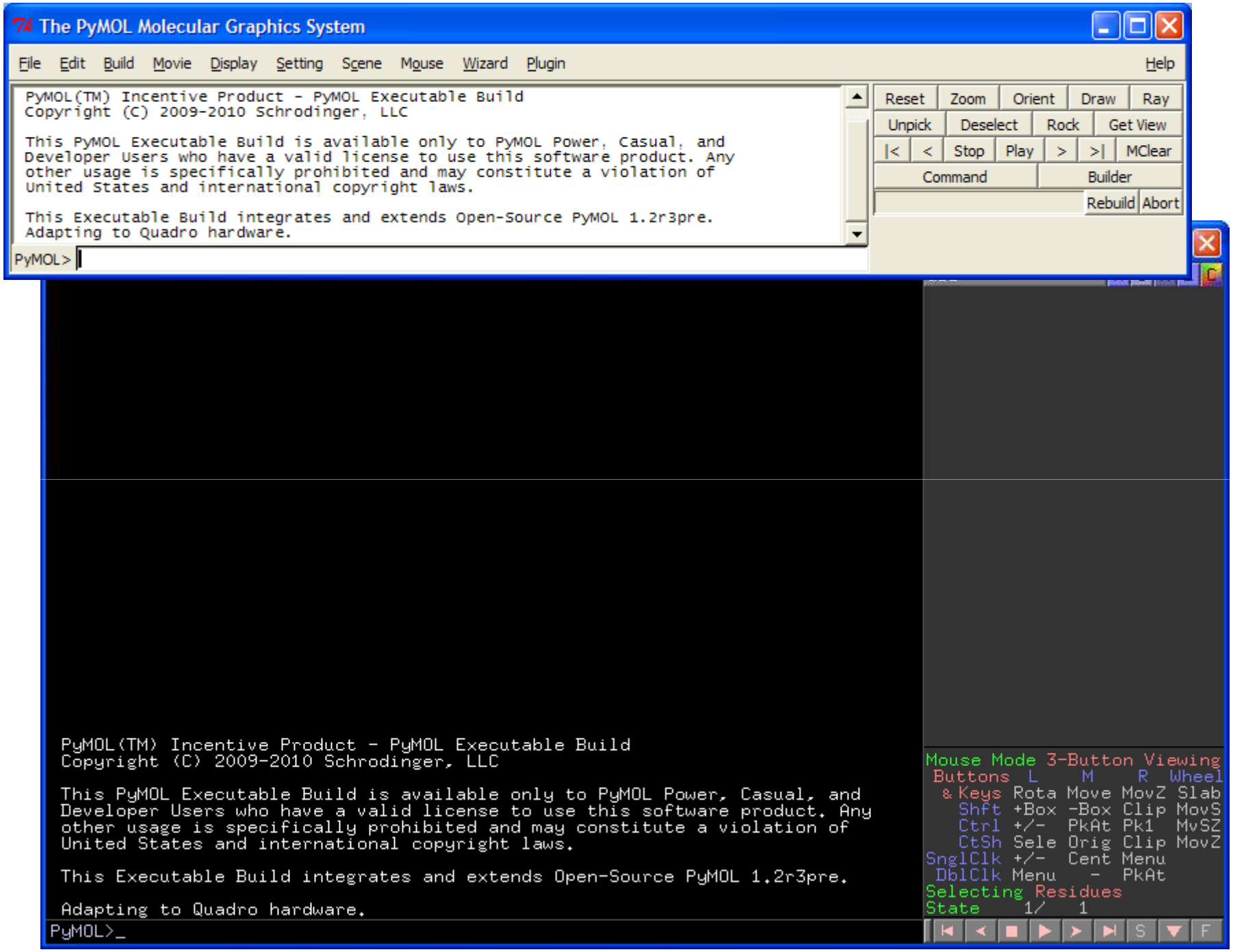
Raccourci de Visualisation

La fenêtre de contrôle



La fenêtre de contrôle




The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
PyMOL(TM) Incentive Product - PyMOL Executable Build
Copyright (C) 2009-2010 Schrodinger, LLC
This PyMOL Executable Build is available only to PyMOL Power, Casual, and
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other usage is specifically prohibited and may constitute a violation of
United States and international copyright laws.
This Executable Build integrates and extends Open-Source PyMOL 1.2r3pre.
Adapting to Quadro hardware.
PyMOL>
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder
Rebuild Abort
PyMOL(TM) Incentive Product - PyMOL Executable Build
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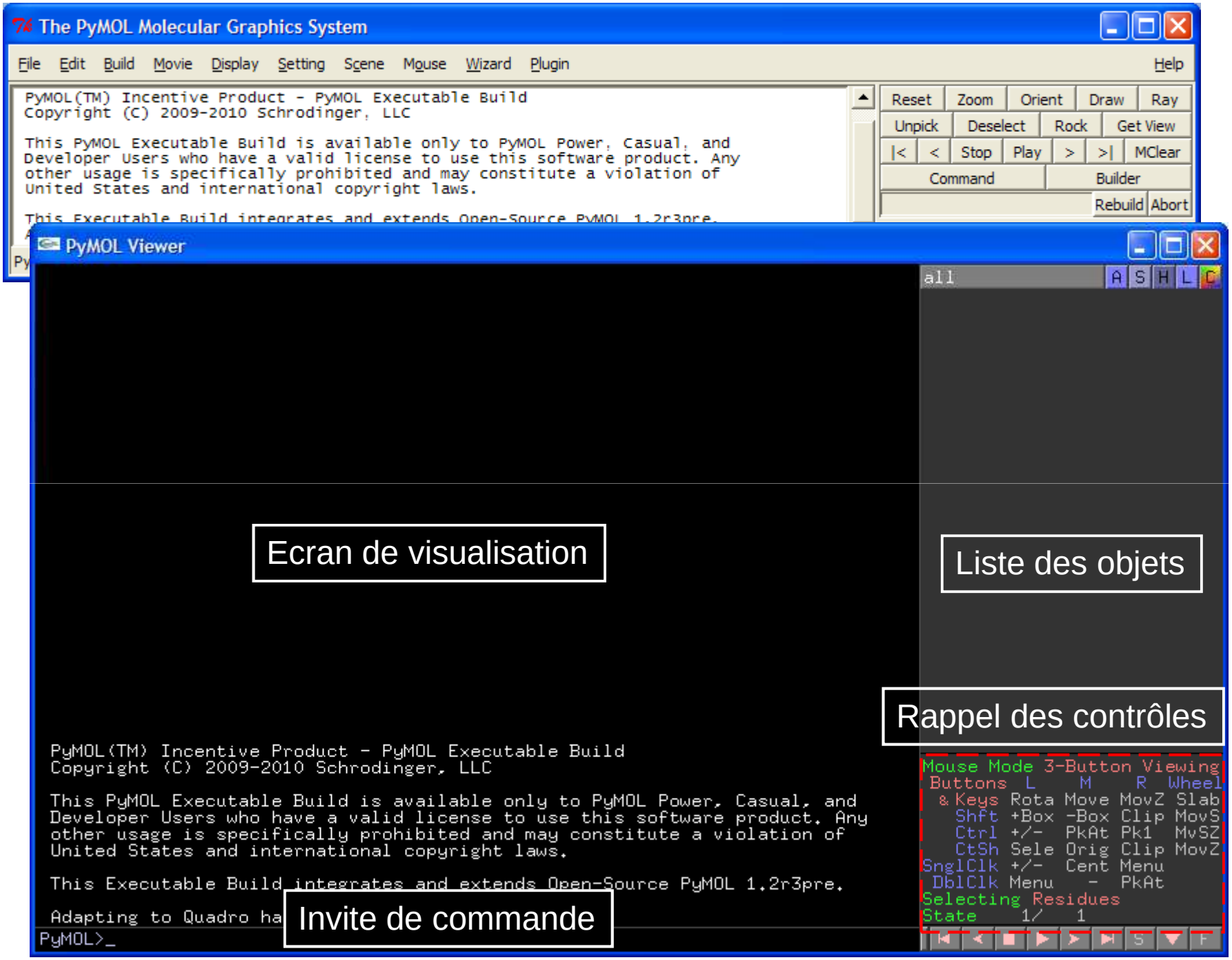
This Executable Build integrates and extends Open-Source PyMOL 1.2r3pre.
Adapting to Quadro hardware.
PyMOL>_
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
S F


The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
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Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder
Rebuild Abort
PyMOL Viewer
all
A S H L C
Ecran de visualisation
Liste des objets
Rappel des contrôles
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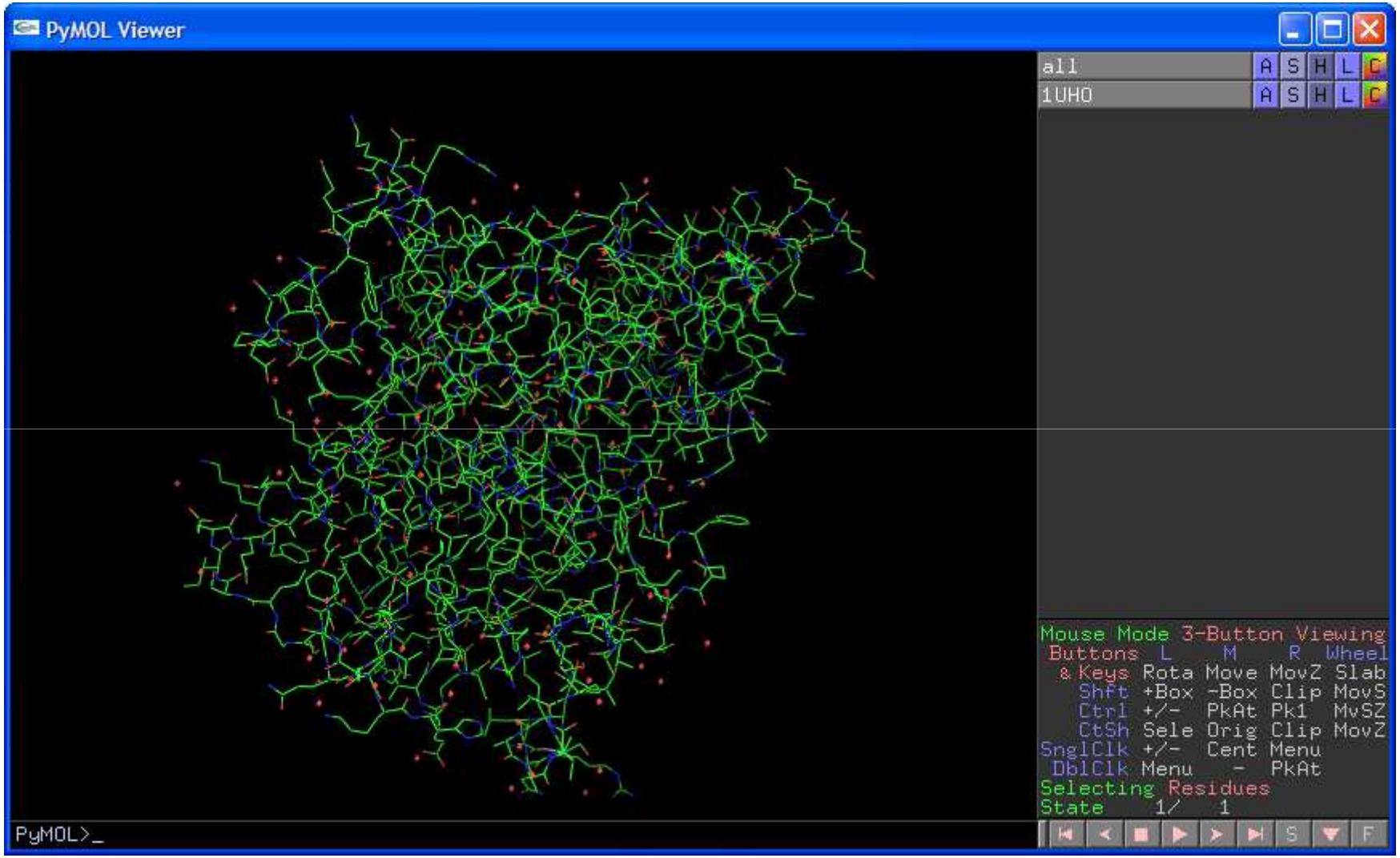
This Executable Build integrates and extends Open-Source PyMOL 1.2r3pre.
Adapting to Quadro ha
Invite de commande
PyMOL>_
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
S

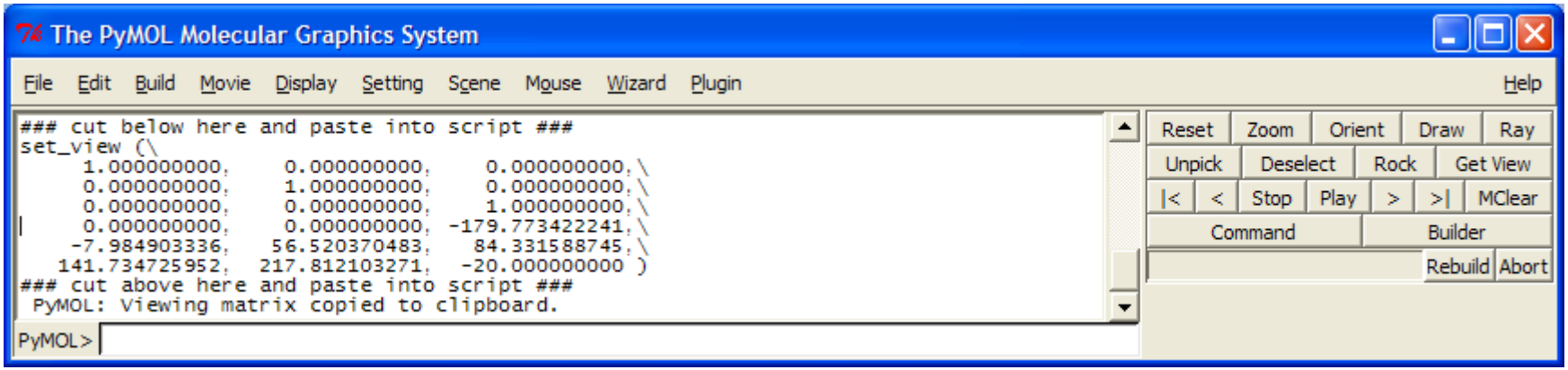
Load 1HUO ou fetch 1HUO

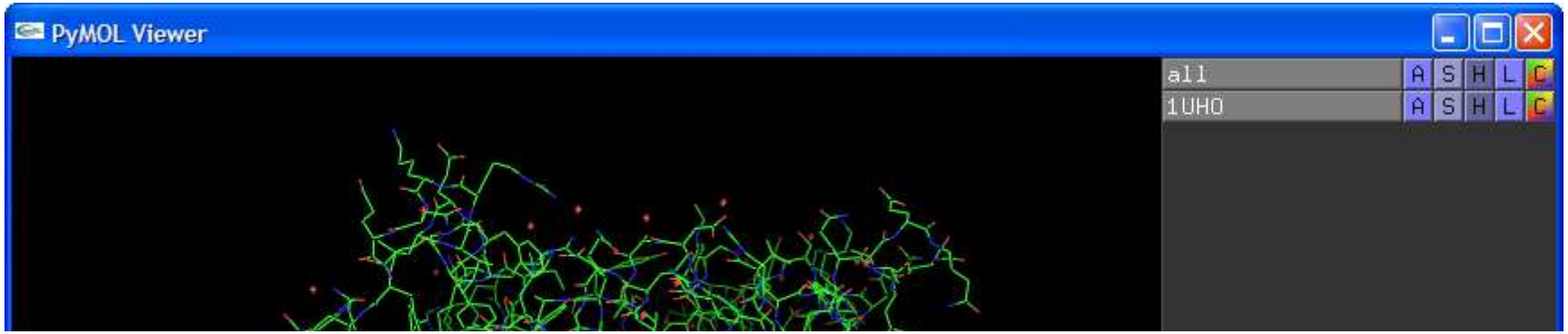


Familiarisation avec la souris

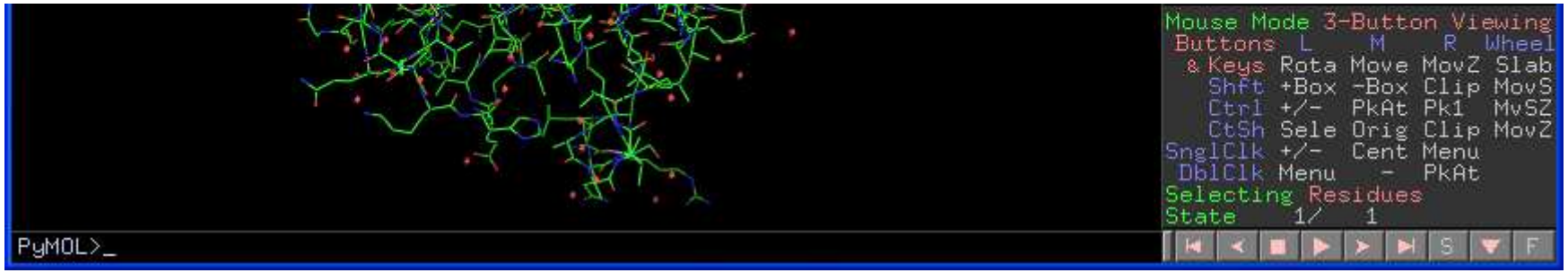
Tableau 2.1. Utilisation de la souris

	boutons de la souris		
Boutons et touches	**Gauche**	**Milieu**	**Droite**
Aucun	Rotation libre	Translation axes x,y	Translation axe z (zoom)
Shift	Agrandir une sélection	Supprimer une sélection	Déplacement du plan de coupe
Ctrl	Inverser la sélection	Sélection de type *PkAt*	Sélection de type *Pk1*
Shift+Ctrl	Sélection d'un résidu	Centrer un atome	Menu de contrôle
double-clic	Menu de contrôle	Centrer un atome	Sélection de type *PkAt*

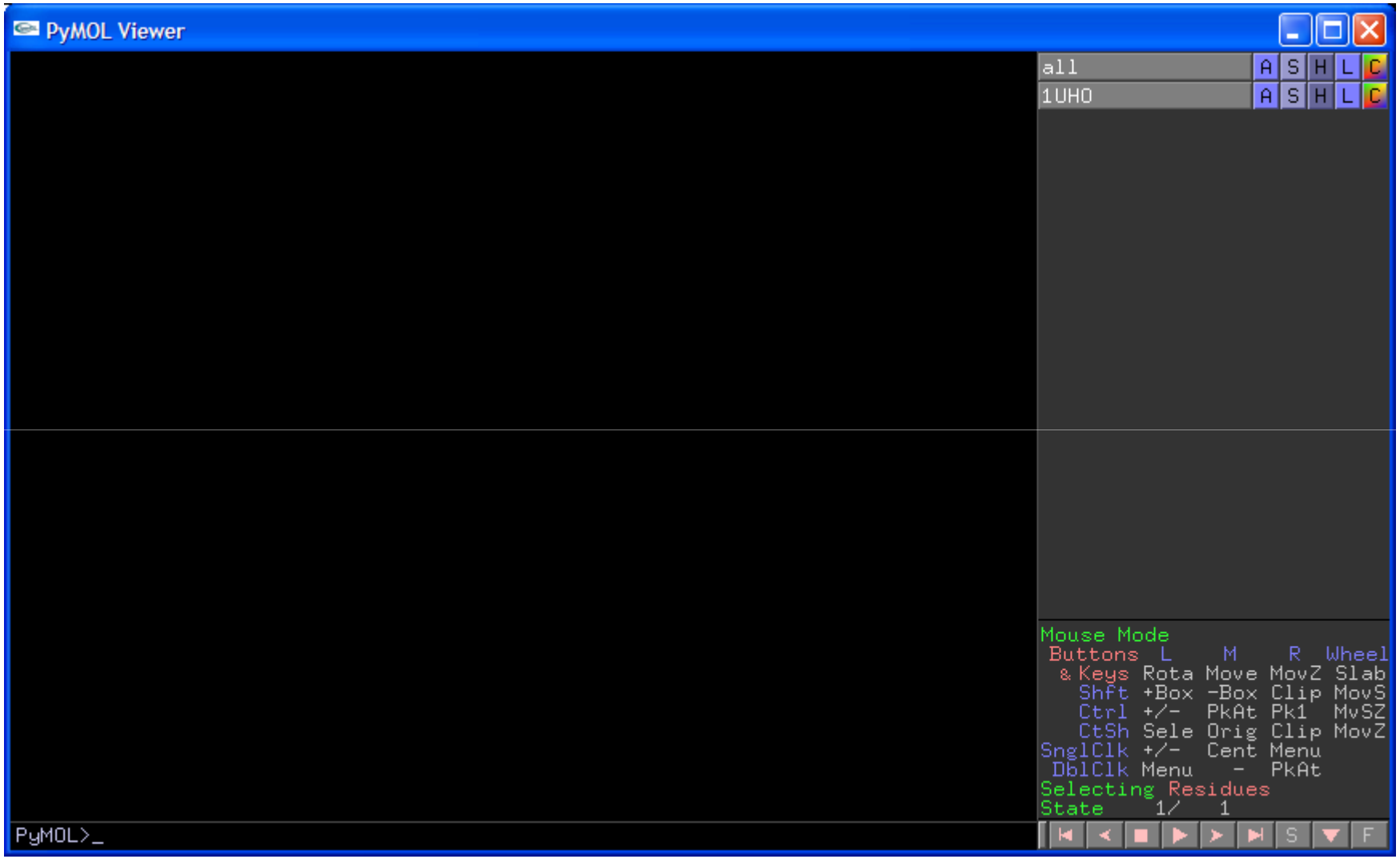




- A (Actions) : ce menu contient toutes les actions qui peuvent être réalisées sur les objets (zoom, alignement, duplication, suppression/ajout des atomes d'hydrogène, ...) ;
- S (Show) : ce menu permet de choisir un ou des styles de visualisation à appliquer à la molécule ;
- H (Hide) : ce menu permet de choisir un ou des styles de visualisation à ne plus appliquer à la molécule ;
- L (Labels) : ce menu permet d'ajouter certains labels sur l'objet, tels que le nom des atomes, des résidus, ... ;
- C (Color) : ce menu permet de changer le style de colorisation de l'objet.

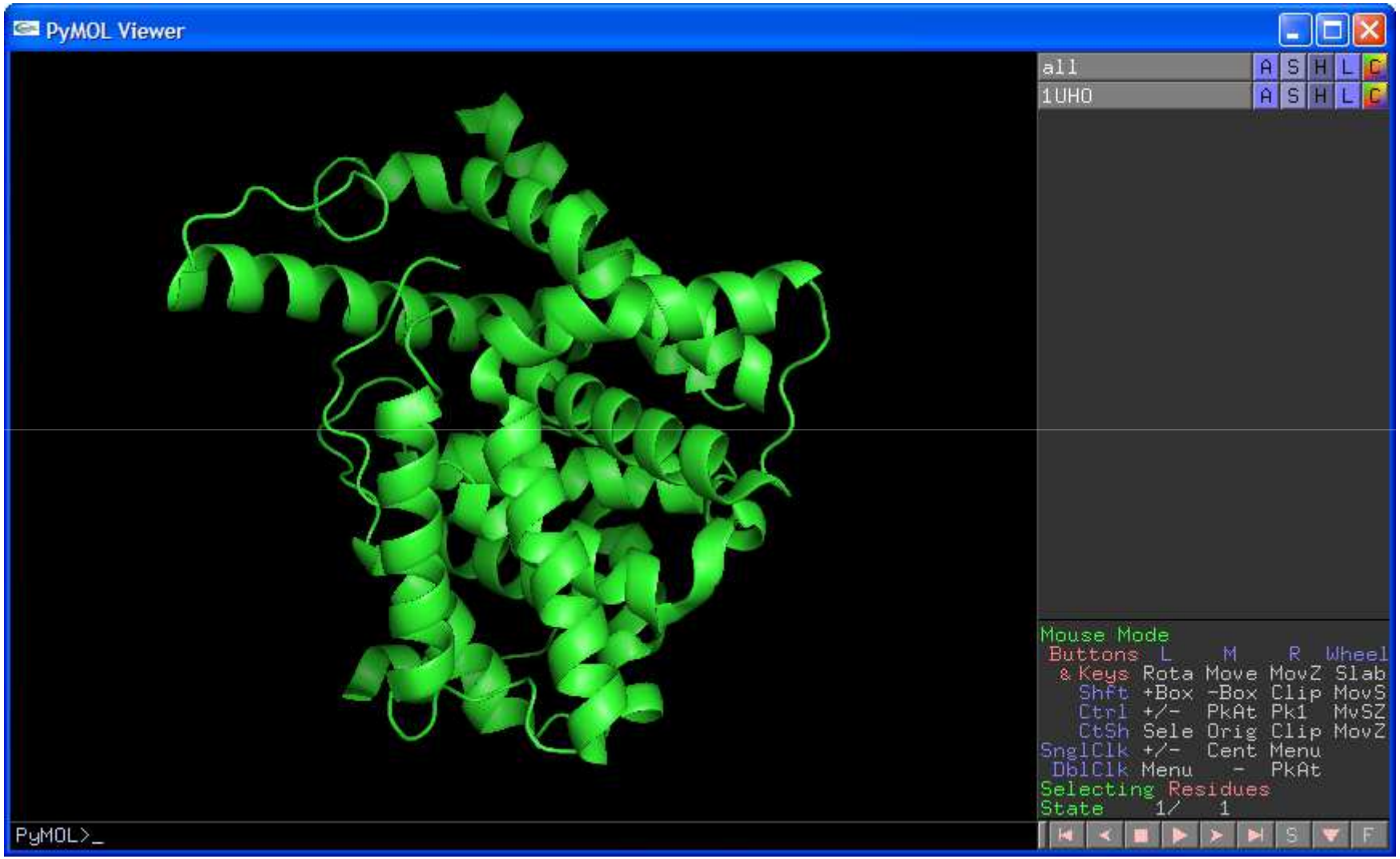


H everything



hide everything

S cartoon



show cartoon, 1huo

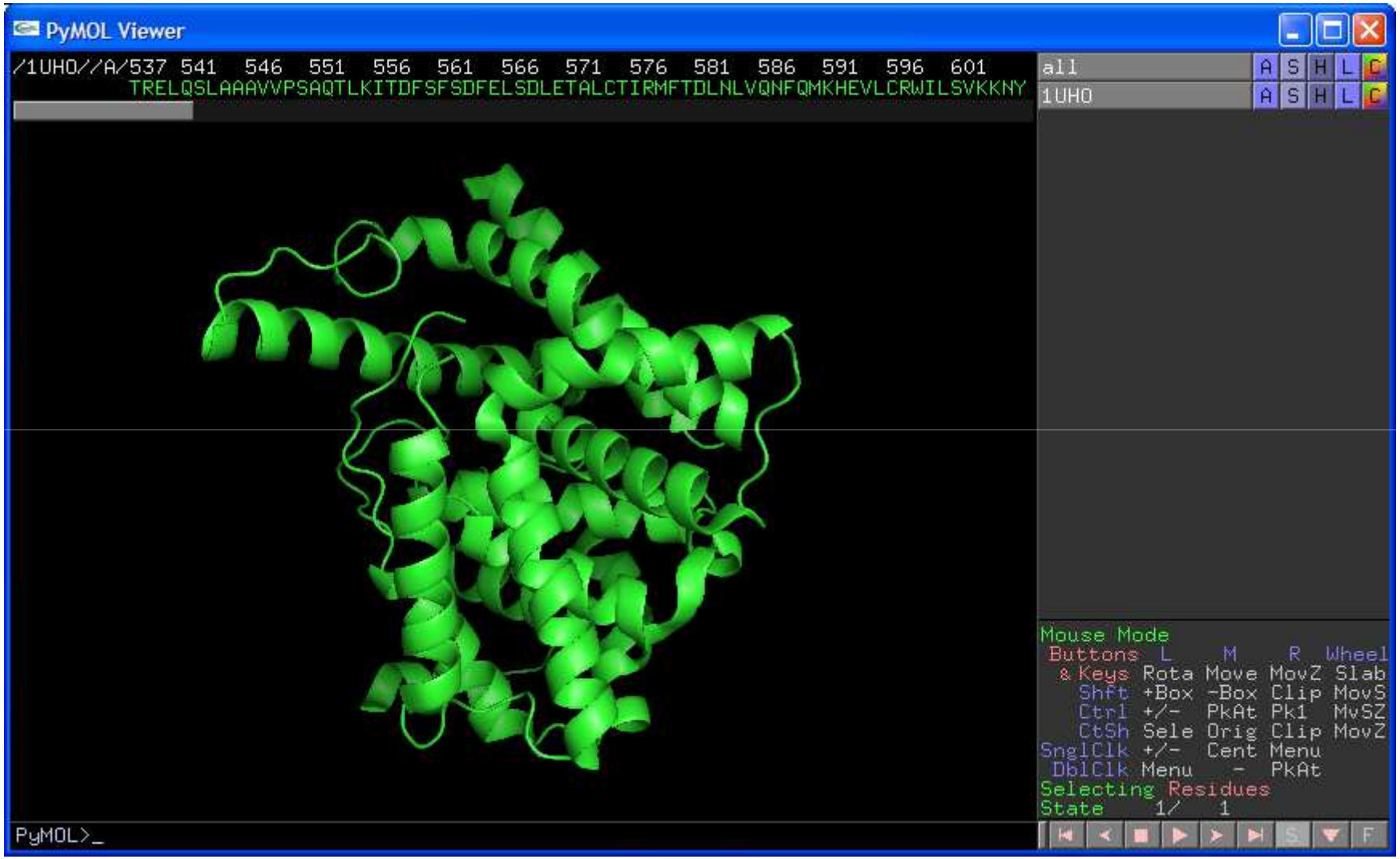
Show/hide [representation [, selection]]

representation =

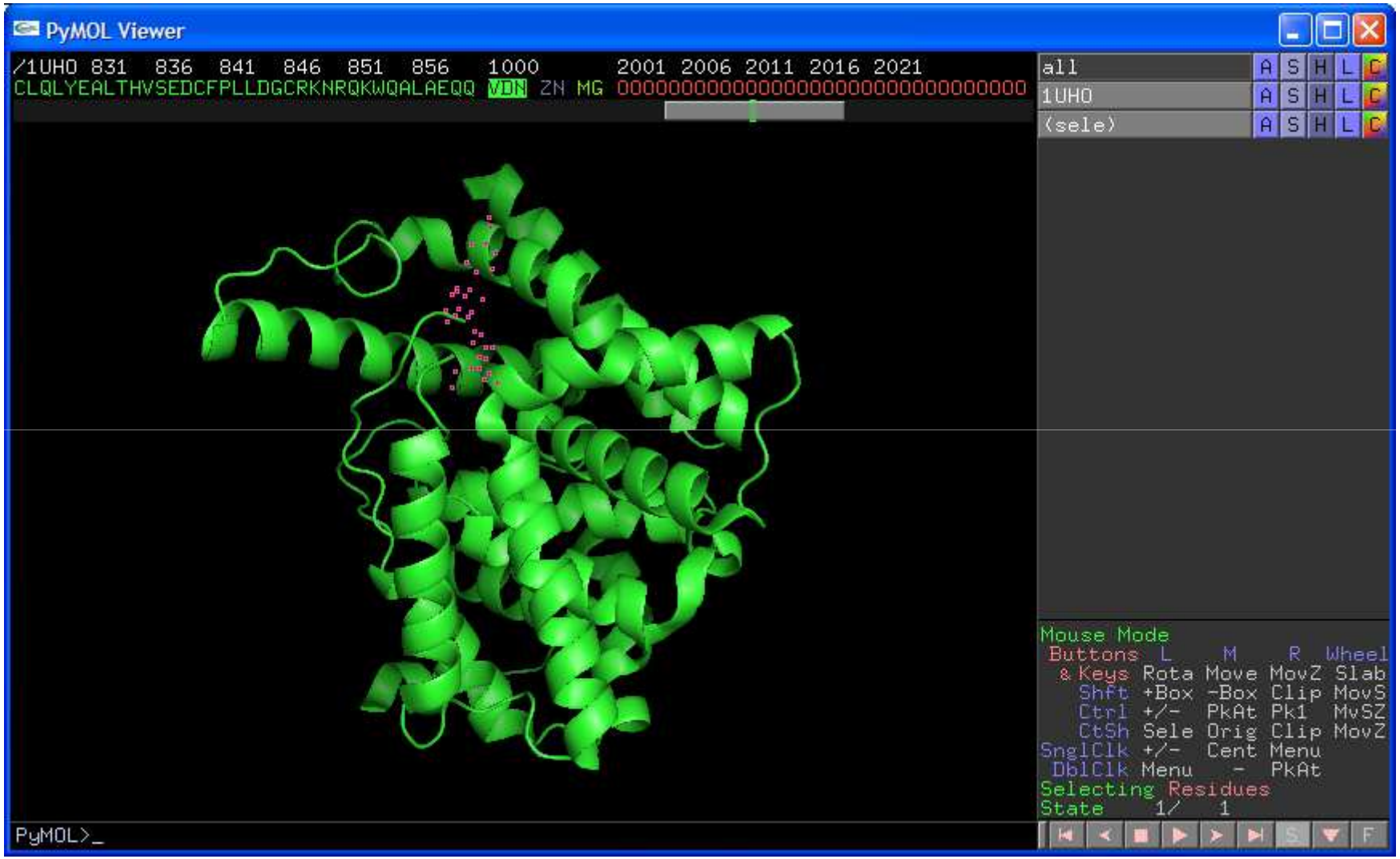
angles	cgo	ellipsoids	lines	*ribbon*	surface
callback	dashes	everything	mesh	slice	
cartoon	dihedrals	extent	nb_spheres	spheres	
cell	dots	labels	nonbonded	sticks	

Tableau 2.2. Les différents styles de visualisation

Style	Effet
lines	Affichage de l'objet avec des lignes fines
nonbonded	Affichage des éléments seuls d'un objet (comme l'oxy-gène de l'eau dans les fichiers PDB)
sticks	Affichage de l'objet avec des bâtons
ribbon	Affichage de la protéine sous la forme d'un fil
cartoon	Représentation de la protéine par un ruban plat pour les feuillets, un ruban en hélice pour les hélices et un fil pour les autres zones
labels	Affichage des labels
cell	Affichage de la cellule cristallographique
dots	Représentation de la surface de van der Waals de chaque atome par un nuage de point
spheres	Représentation de la surface de van der Waals de chaque atome en dure
nb_spheres	Représentation des éléments seuls (non liés) par des sphères
mesh	Représentation de la surface de l'objet par un réseau de fils
surface	Affichage de la surface de l'objet avec une texture pleine
main chain	Représentation de la chaîne principale de la protéine
side chain	Représentation des chaînes secondaires de la protéine


PyMOL Viewer
/1UHO//A/537 541 546 551 556 561 566 571 576 581 586 591 596 601
TRELQSLAAAVVPSAQTLKITDFSFSDFELSDLETALCTIRMFTDLNLVQNFQMKHEVLCRWILSVKKNY
all
1UHO
Mouse Mode
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_

On sélectionne le residue 1000 « VDN »



Un nouvel object (sele)

Sélection des objets

Display sequence
Sequence mode
set seq_view_label_mode = 0,1,2,3

select object-name/segi_id/chain_id/resi_id/name_id/

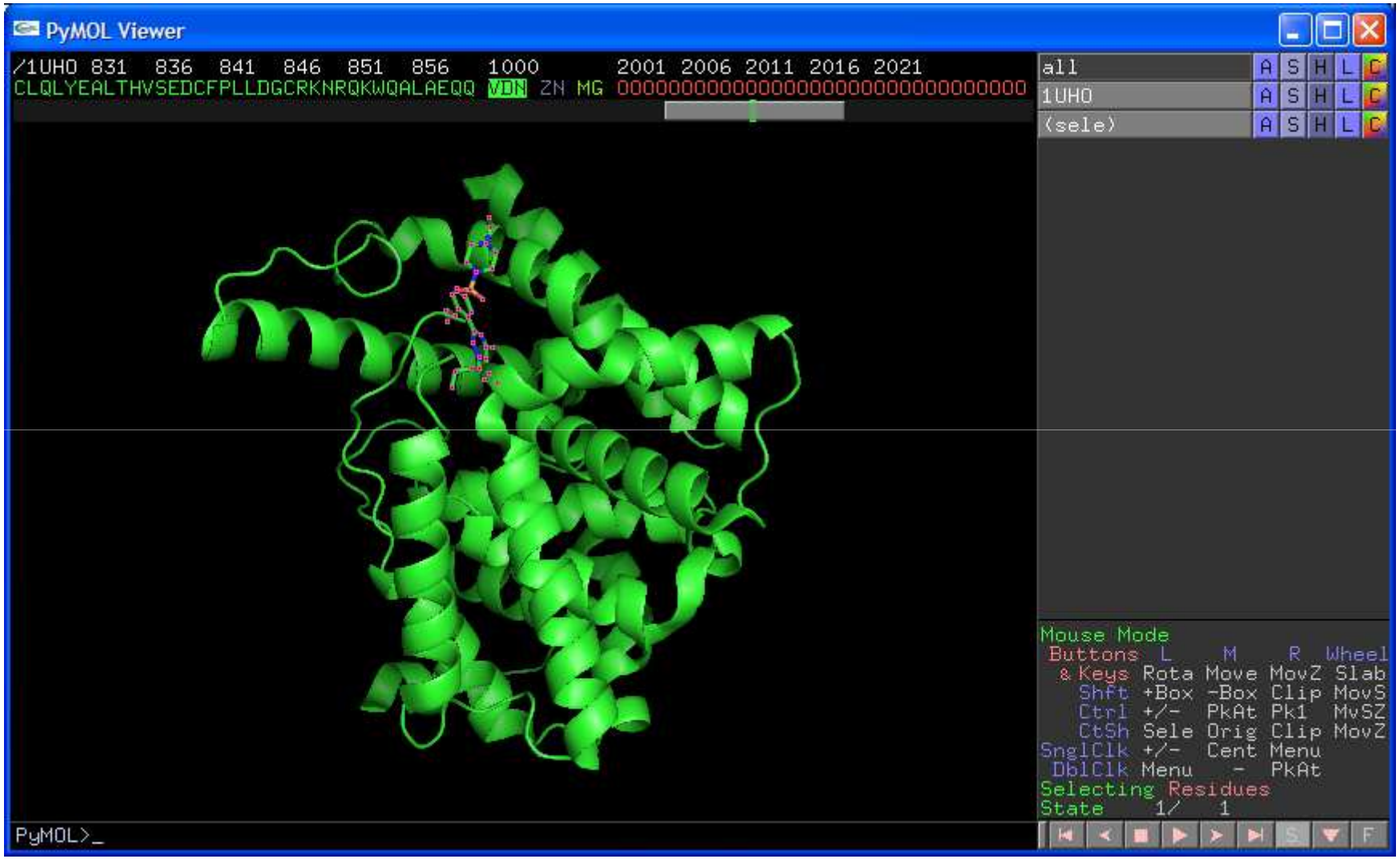
select object-name and name C8 and resi 1 and resname ALA
and chain A and symbol C

resi 10-12
resi 10+12

hide/show cartoon, !(c. A) = hide cartoon, not chain A

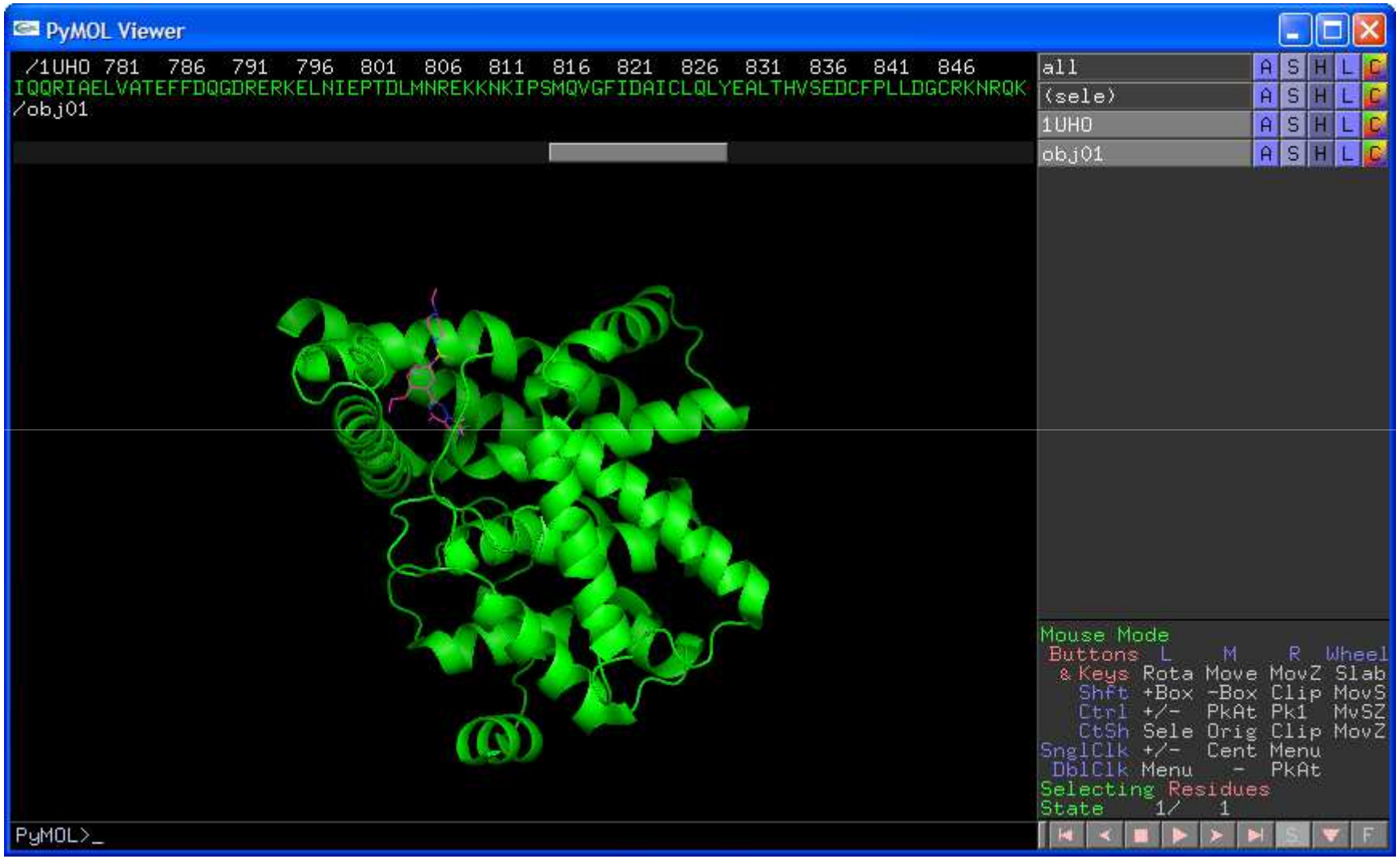
hide/show everything (type de représentations), selection
hide all (objets)
everything = line+sticks+ribbon+cartoon+spheres

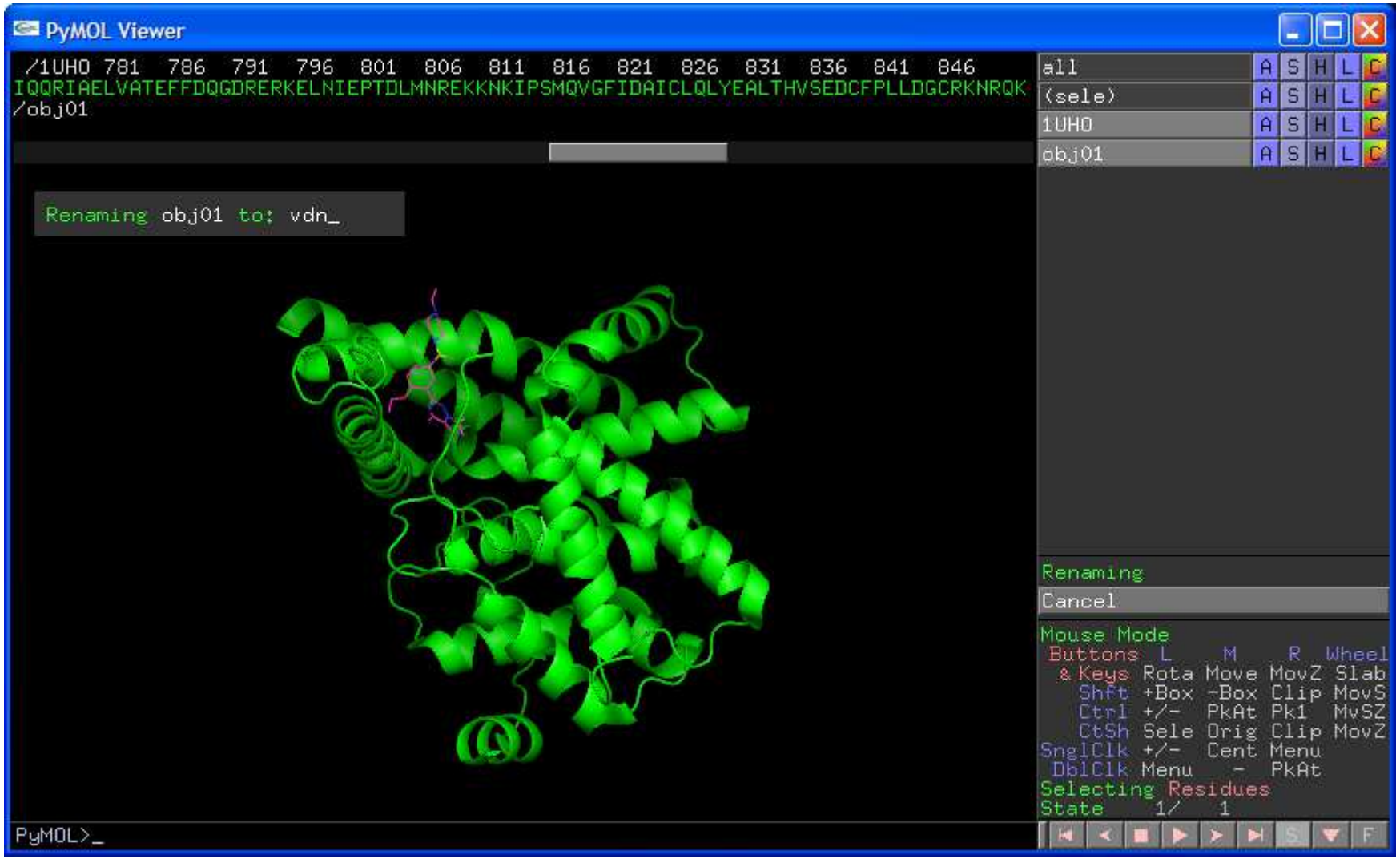
Représentation stick du residue 1000 « VDN » (sele)



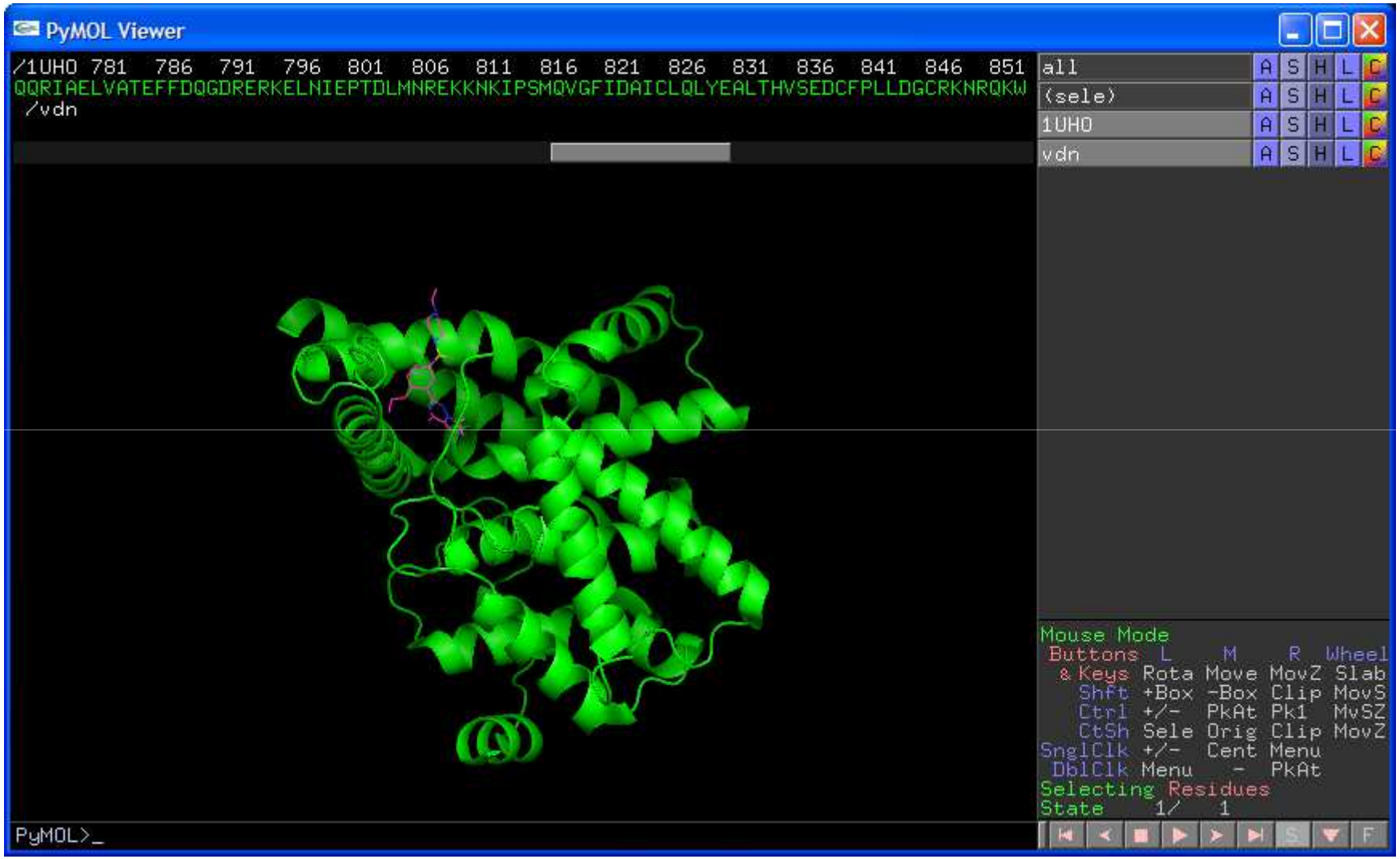
(sele) copy to object obj01 est créé

rename vdn

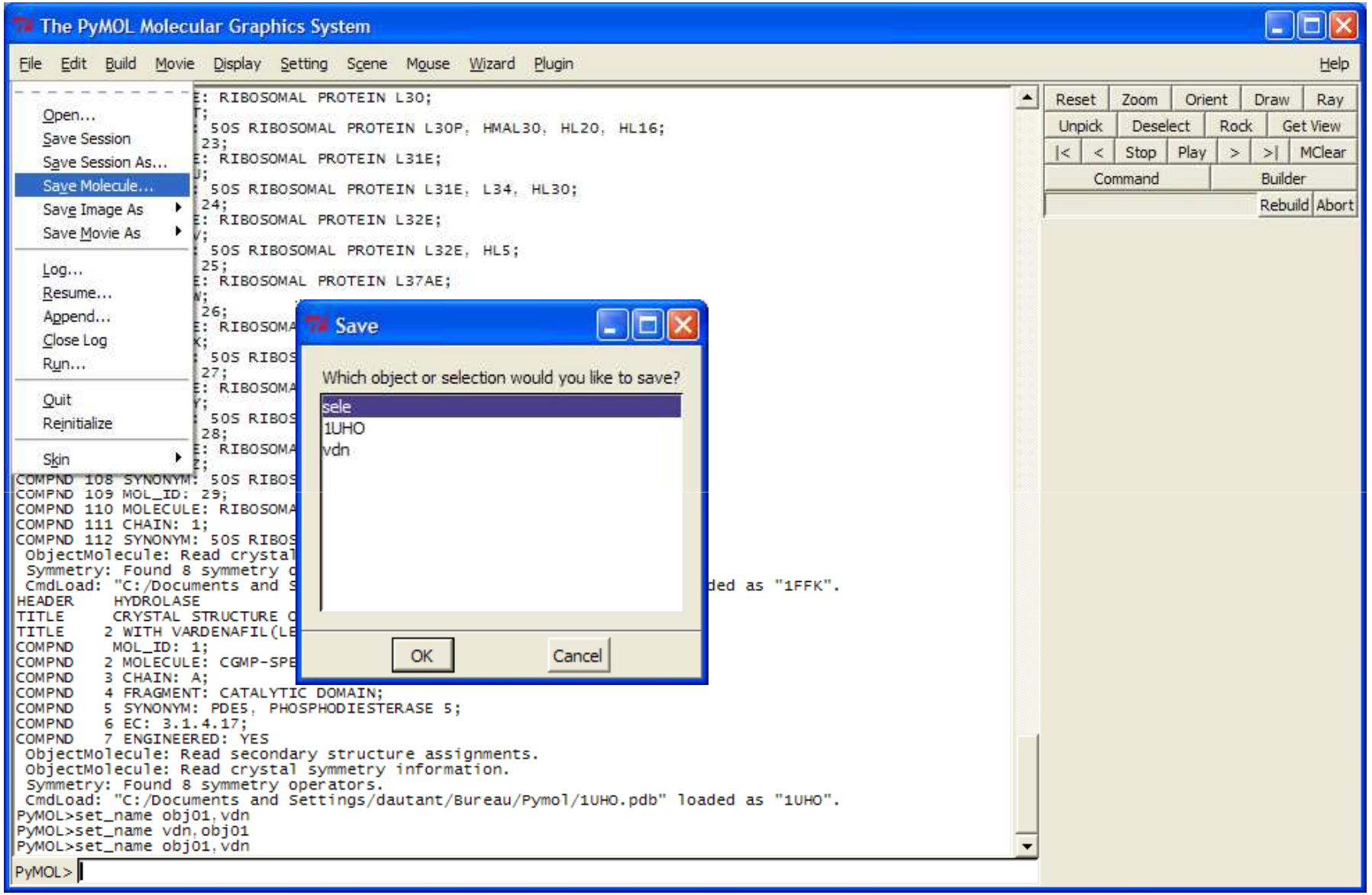



PyMOL Viewer
/1UH0 781 786 791 796 801 806 811 816 821 826 831 836 841 846
IQQRIAELVATEFFDQGDRERKELNIEPTDLMNREKKNKIPSMQVGFIDAICLQLYEALTHVSEDCFPLLDGCRKNRQK
/obj01
Renaming obj01 to: vdn_
all
(sele)
1UH0
obj01
Renaming
Cancel
Mouse Mode
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_

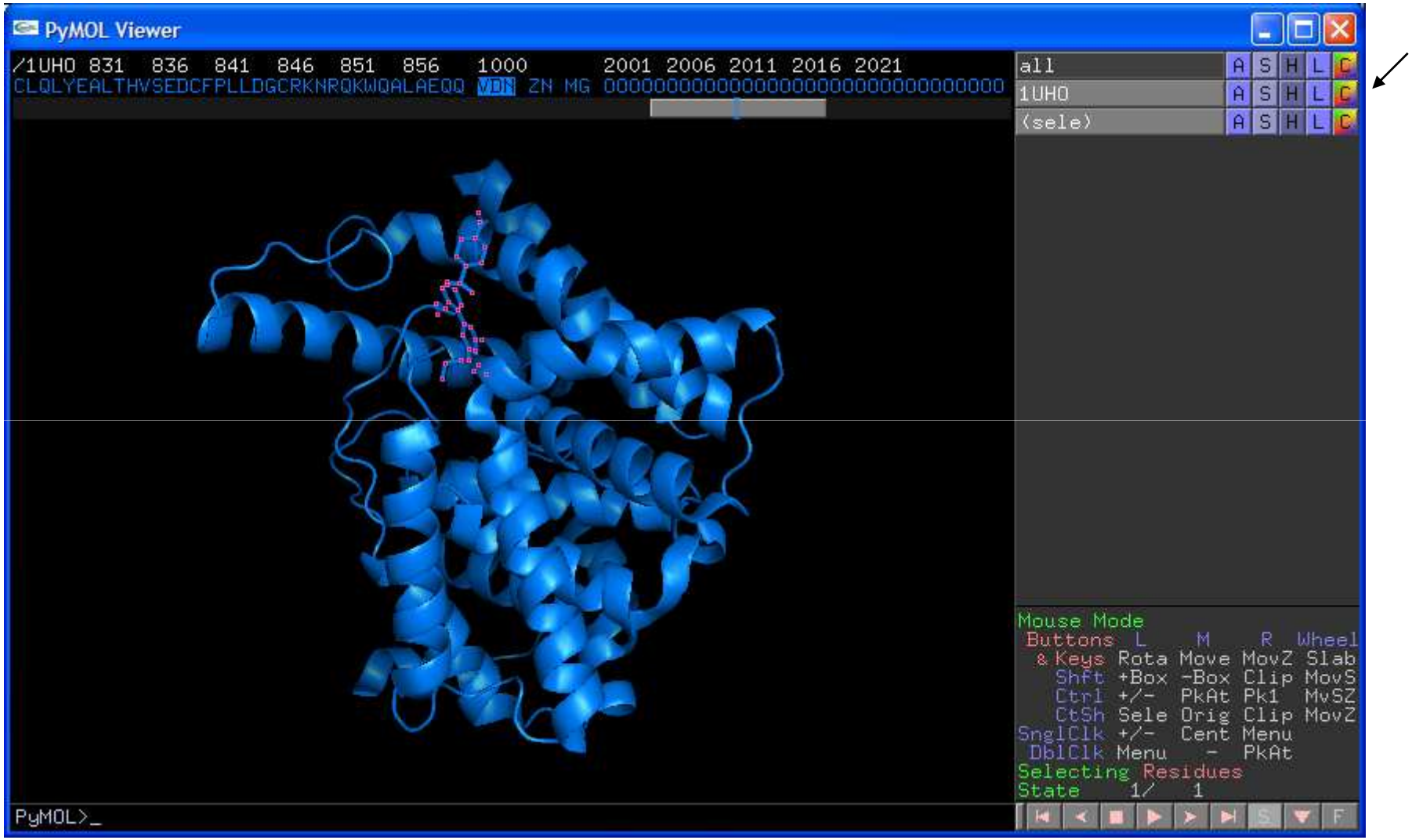
Deux objets



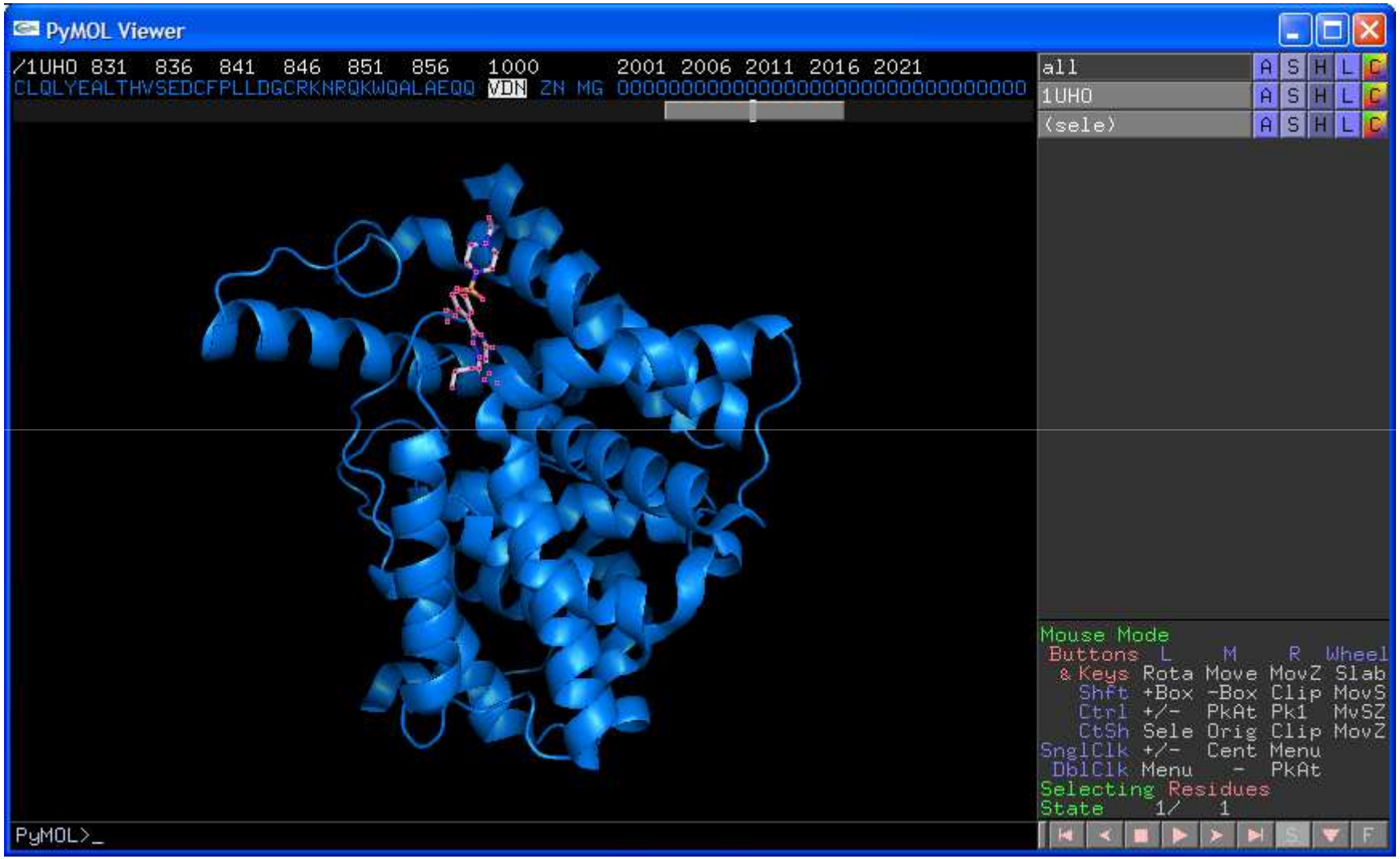
Nous voulons sauvegarder l’objet (la molécule) vdn


The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
Open...
Save Session
Save Session As...
Save Molecule...
Save Image As
Save Movie As
Log...
Resume...
Append...
Close Log
Run...
Quit
Reinitialize
Skin
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
|< < Stop Play > >| MClear
Command Builder
Rebuild Abort
Save
Which object or selection would you like to save?
sele
1UHO
vdn
OK
Cancel
COMPND 108 SYNONYM: 50S RIBOS
COMPND 109 MOL_ID: 29;
COMPND 110 MOLECULE: RIBOSOMA
COMPND 111 CHAIN: 1;
COMPND 112 SYNONYM: 50S RIBOS
ObjectMolecule: Read crystal
Symmetry: Found 8 symmetry o
CmdLoad: "C:/Documents and S
HEADER HYDROLASE
TITLE CRYSTAL STRUCTURE O
TITLE 2 WITH VARDENAFIL(LE
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: CGMP-SPE
COMPND 3 CHAIN: A;
COMPND 4 FRAGMENT: CATALYTIC DOMAIN;
COMPND 5 SYNONYM: PDE5, PHOSPHODIESTERASE 5;
COMPND 6 EC: 3.1.4.17;
COMPND 7 ENGINEERED: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 8 symmetry operators.
CmdLoad: "C:/Documents and Settings/dautant/Bureau/Pymol/1UHO.pdb" loaded as "1UHO".
PyMOL>set_name obj01,vdn
PyMOL>set_name vdn,obj01
PyMOL>set_name obj01,vdn
PyMOL>

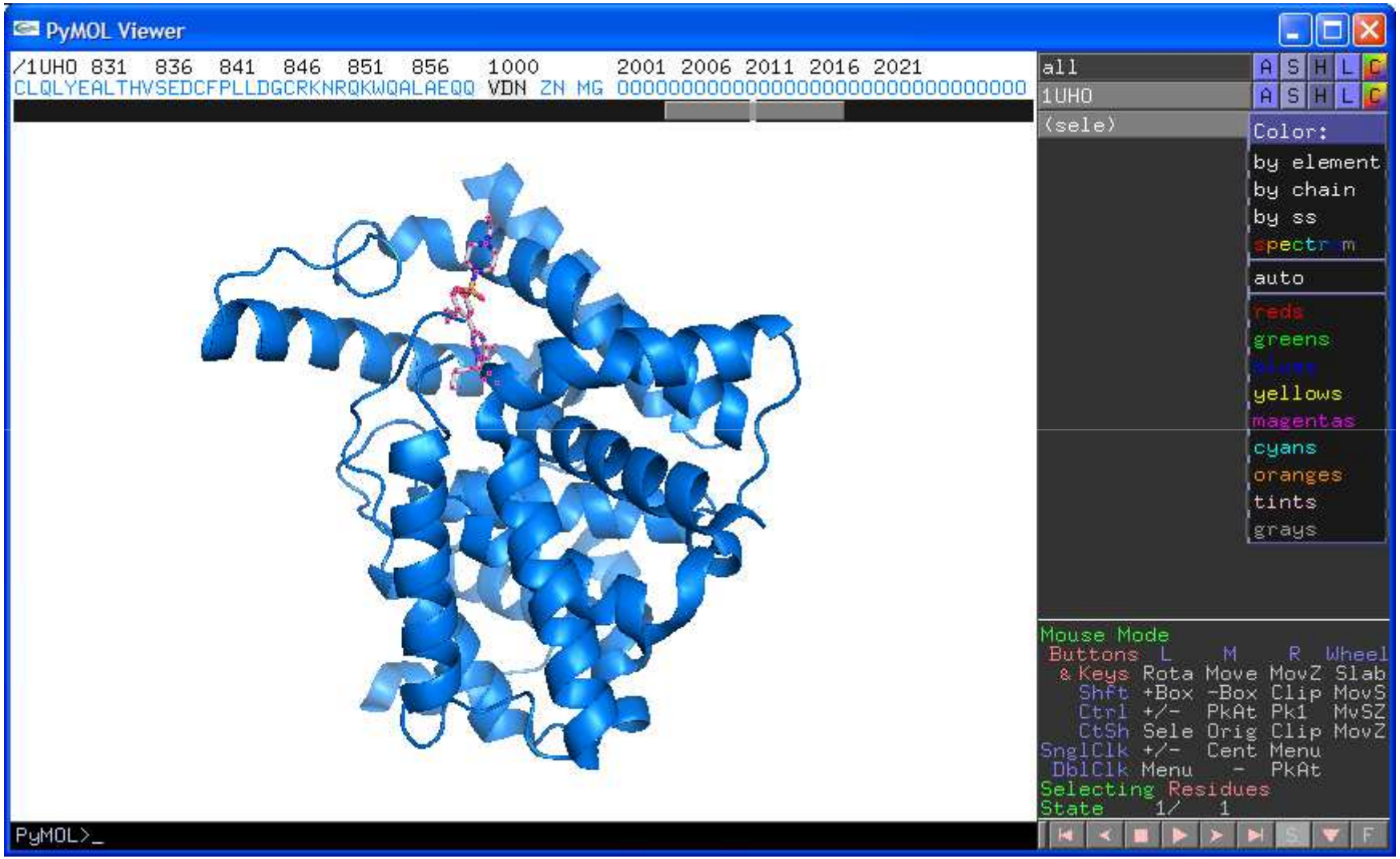
Colorons 1UHO en bleu marine



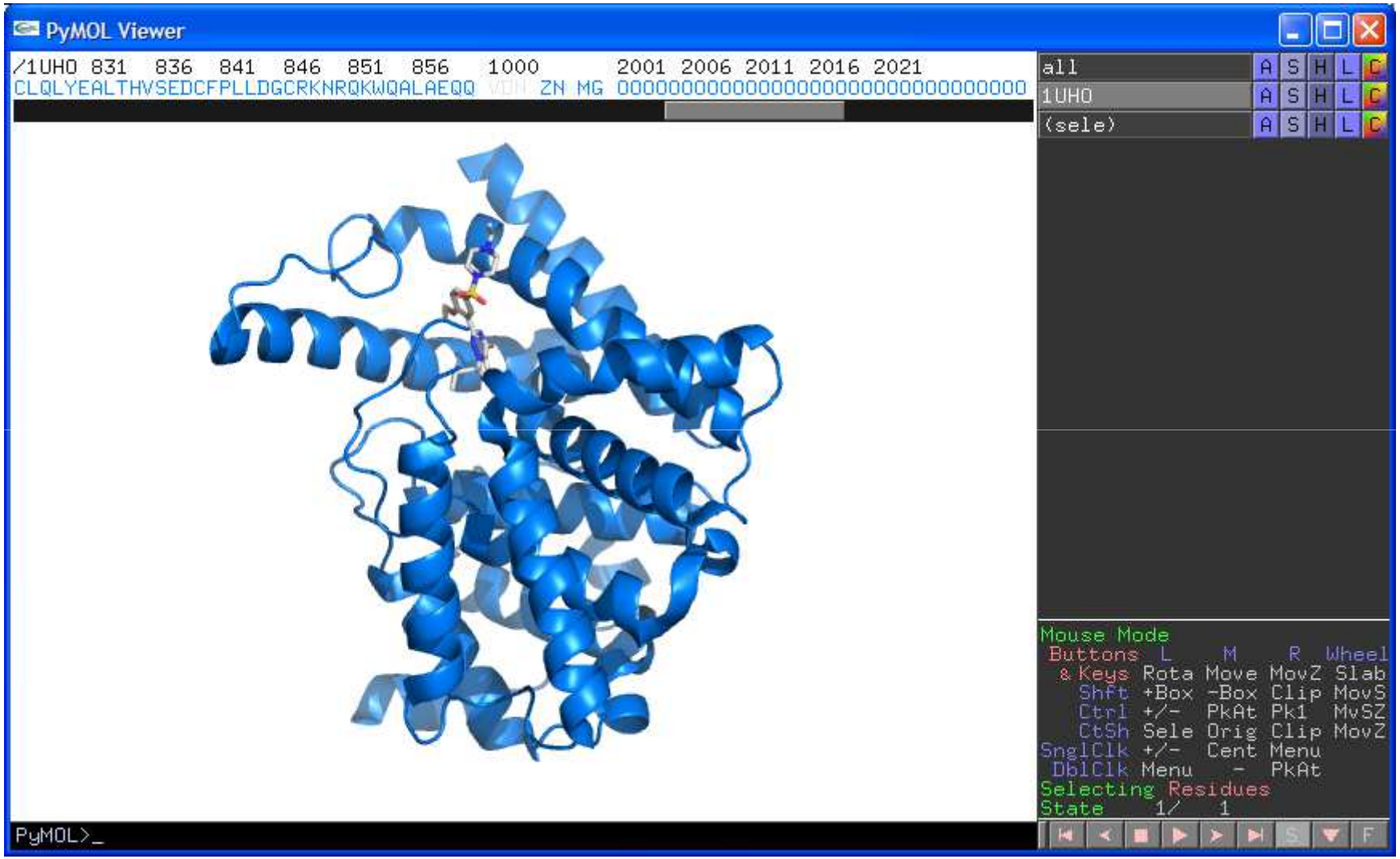
Colorons VDN en color by element



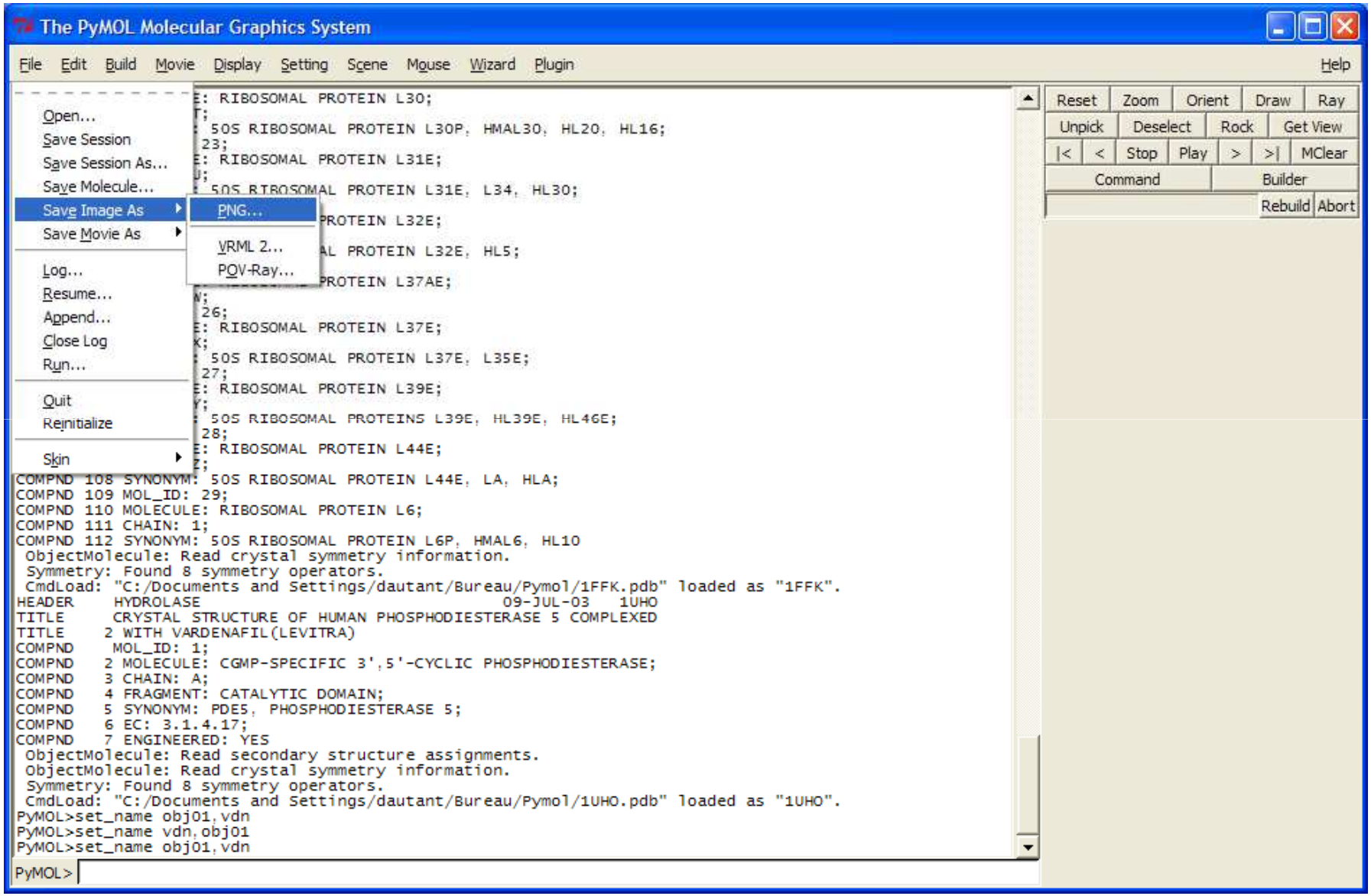
display background white (opaque)
display orthoscopic view



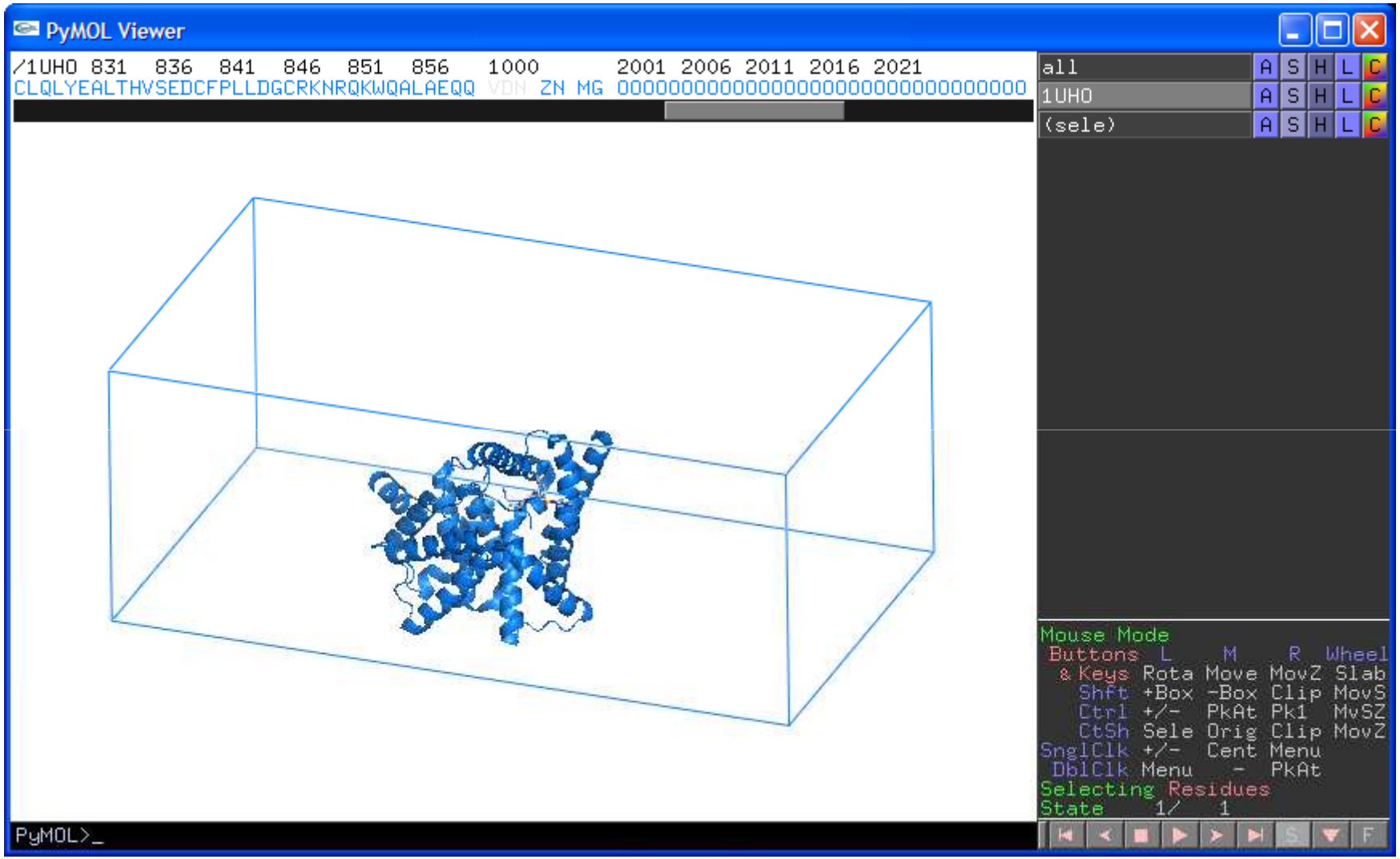
ray


PyMOL Viewer
/1UHO 831 836 841 846 851 856 1000 2001 2006 2011 2016 2021
CLQLYEALTHVSEDCFPLLDGCRKNRQKWQALAEQQ VDN ZN MG OOOOOOOOOOOOOOOOOOOOOOOOOOOOOO
all A S H L C
1UHO A S H L C
(sele) A S H L C
Mouse Mode
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_

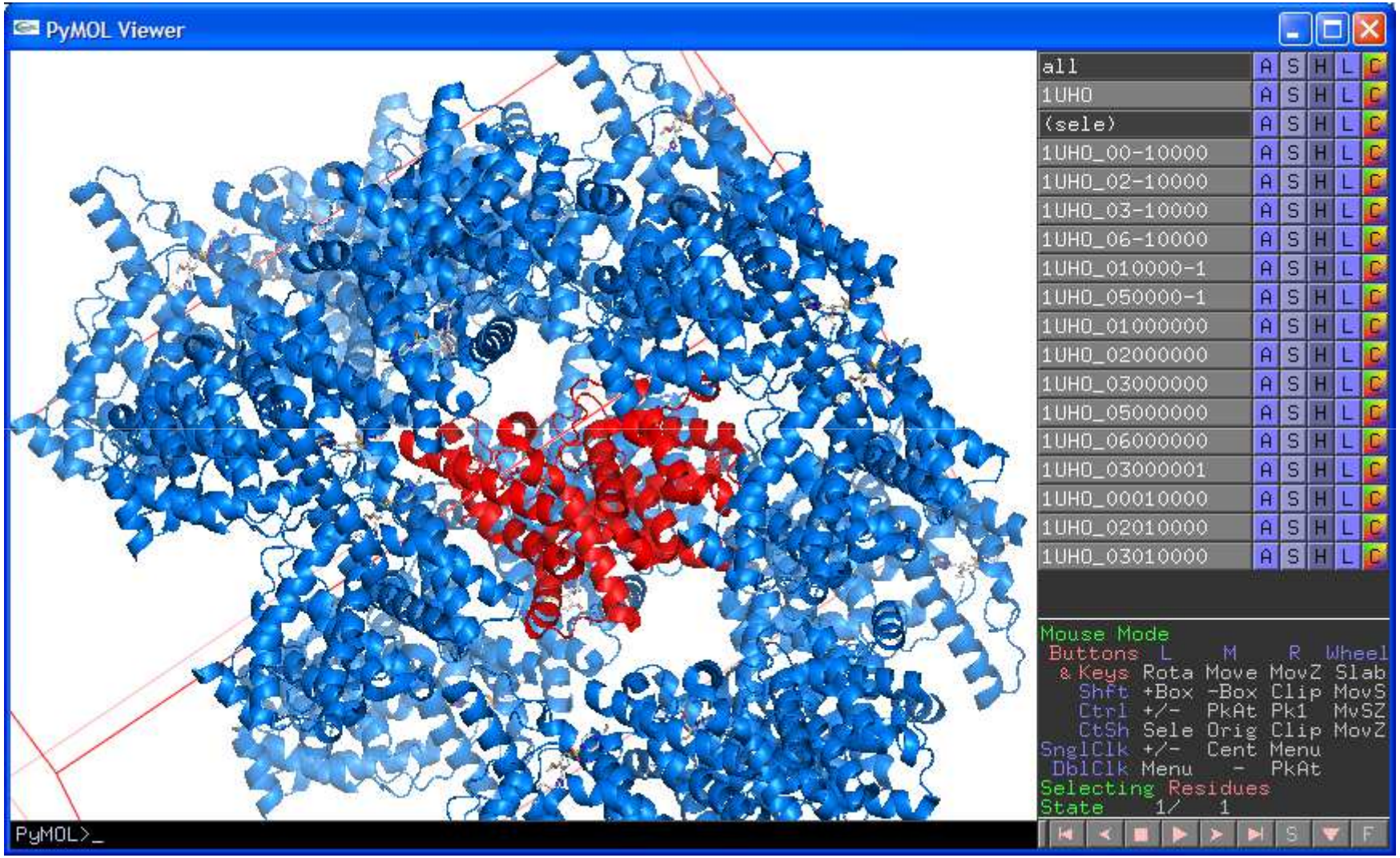
Sauvegarde de l'image au format png



show cell


PyMOL Viewer
/1UHO 831 836 841 846 851 856 1000 2001 2006 2011 2016 2021
CLQLYEALTHVSEDCFPLLDGCRKNRQKWQALAEQQ VDN ZN MG OOOOOOOOOOOOOOOOOOOOOOOOOOOOOO
all A S H L C
1UHO A S H L C
(sele) A S H L C
Mouse Mode
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_

Action generate symmetry_mates within_20_A



delete 1uho_*

Faire du « Ball and stick »

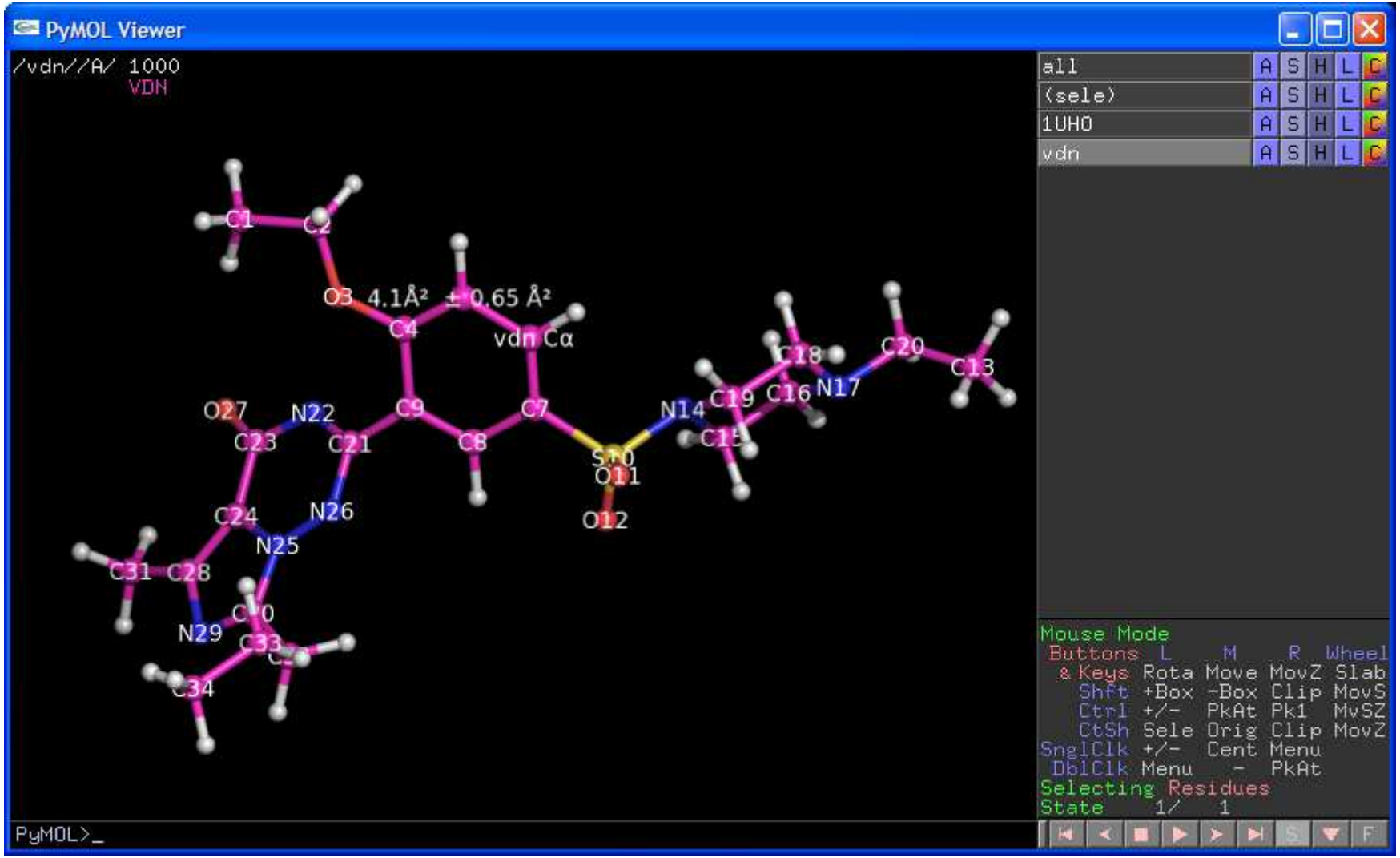
```
h_add
show stick, vdn
show spheres, vdn
set sphere_scale = 0.15
set stick_radius, 0.10

set orthoscopic = 1

png ball-and-stick.png
ls
pwd

# labeling syntax
label [ selection[, expression]]

label vdn and name c6, " vdn "  + u"C\u03b1"
set label_size, 40
set label_position,(2,0,0)
label vdn and name c5, "4.1" + u"\u00c5\u00b2  \u00b1 0.65 \u00c5\u00b2 "
```

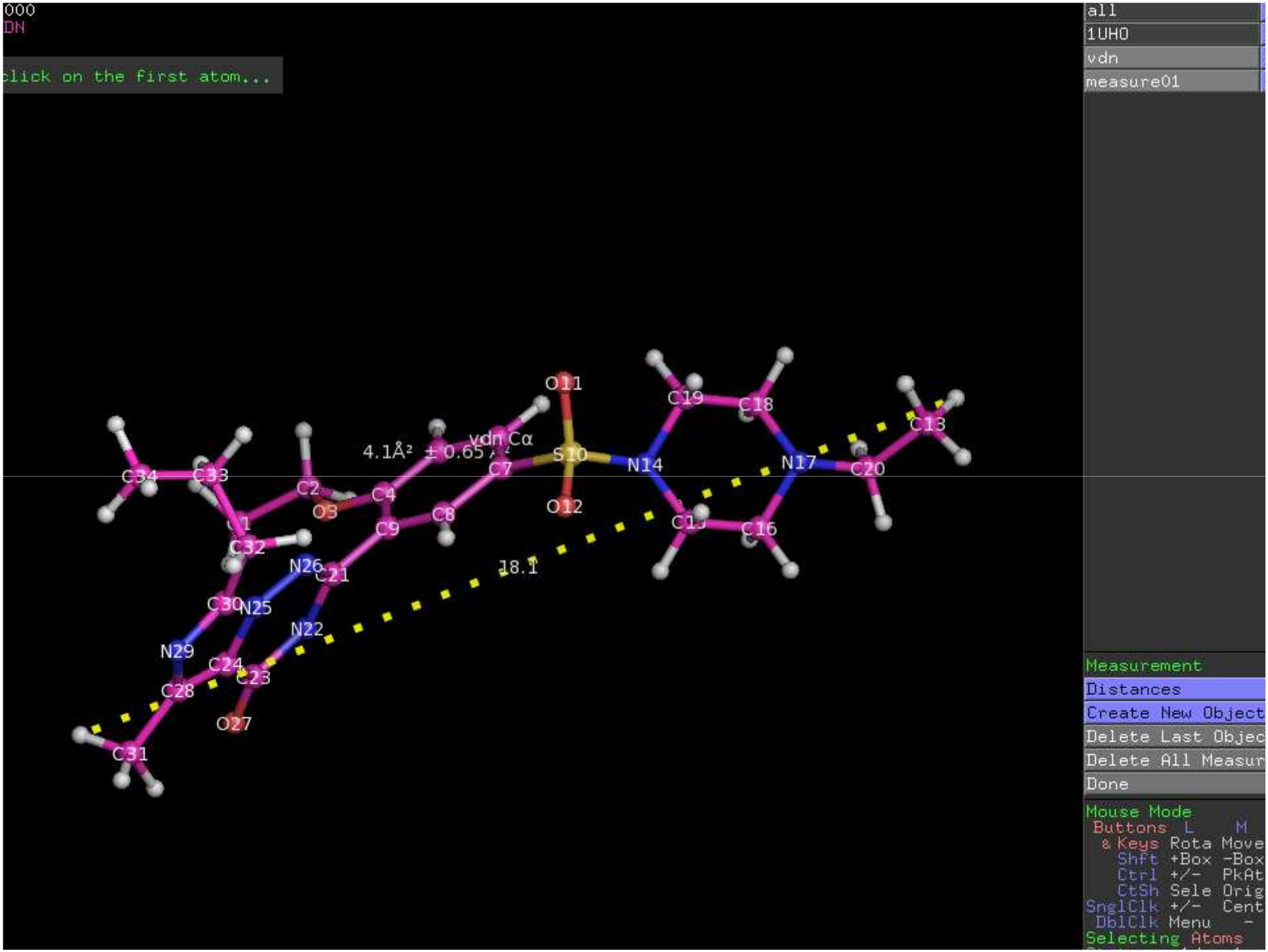

PyMOL Viewer
/vdn//A/ 1000
VDN
O3 4.1Å² ± 0.65 Å²
vdn Cα
C1
C2
C4
C9
C7
C8
O27
N22
C23
C21
C24
N26
N25
C31
C28
N29
C33
C34
N14
C19
C16
N17
C18
C20
C13
S10
O11
O12
all
(sele)
1UH0
vdn
A S H L C
Mouse Mode
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_

Superposer des molécules (pairwise)

align lactame_L, lactame_D and n. O8+C3+N2+C4+C1
RMS = 0.054 (5 to 5 atoms)

Prendre des mesures et les tracer (Utiliser le Wizard)

distance dist_1, atom1, atom2, cutoff = 2.5
angle angle_1, angle_1, sele1, sele2, sele3
dihedral dihe_1, atom1, atom2, atom3, atom4


000
DN
click on the first atom...
all
1UHO
vdn
measure01
O11
C19
C18
C13
vdn Cα
4.1Å² ± 0.65
S10
N14
N17
C20
C34
C33
C2
C4
C7
O3
O12
C8
C9
C32
N26
C21
18.1
C30
N25
N22
N29
C24
C23
C28
O27
C31
Measurement
Distances
Create New Object
Delete Last Objec
Delete All Measur
Done
Mouse Mode
Buttons L M
& Keys Rota Move
Shft +Box -Box
Ctrl +/- PkAt
CtSh Sele Orig
SnglClk +/- Cent
DblClk Menu -
Selecting Atoms

Les formats supportés

Entrée	Sortie
Ils sont très nombreux	pse pml pdb png

Les scripts 1huo.pml

```
load 1UHO.pdb, 1UHO
hide everything, 1UHO
show cartoon, 1UHO
color grey, 1UHO
select vdn,(resn VDN)
show sticks, (vdn)
color wheat, (elem c & vdn)
color red, (elem o & vdn)
color blue, (elem n & vdn)
color orange, (elem s & vdn)
select voisins,(vdn around 6)
delete vdn
hide everything, (voisins)
show surface, (voisins)
color marine, (voisins)
rotate x, 140, (1UHO)
hide everything,(resi 663,664)
zoom (voisins)
delete voisins
ray
```

Rendez vous à Bordeaux

AFC 2013

2-5 juillet 2013

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