DESCRIPTION
`count_frames` is an API-only function which returns the number of frames defined for the PyMOL movie.
PYMOL API
```
cmd.count_frames()
```

Typically the API-only command would only be useful to a programmer.

4 *PyMol - Exercise Q*: Multistate PDB files (NMR) – animation and relative movement

NMR solves structure in solution rather than within a locked crystal. Therefore there are multiple solutions to solving the structure due to some of the movements of the atoms in solution. Typically, NMR structures are published as a set of 10, 20 or 30 plausible structures under one PDB accession file. For example the NMR structure 1NYZ contains 20 structures. However searching for this structure within the PDB site will present the updated version with the new accession name 1sy4 containing only 12 structures also called models or states.

✔ **TASK**

√ - **Open** a web **browser** to the PDB site http://www.rcsb.org/pdb/
√ - **search** and retrieve **1sy4**
(on the left side blueish panel, **click on Download Files**, then on PDB text and a file named 1SY4.pdb will be created on the desktop.)

If you open the PDB file with a word processor, you can observe that each structural state starts with the keyword `MODEL` and is separated from the next with the keyword `ENDMDL`.

```
MODEL        1
ATOM      1  O5'   G A   1     -11.545 -12.549   4.261  1.00  0.00           O
ATOM      2  C5'   G A   1     -12.281 -11.830   5.254  1.00  0.00           C
//
ATOM    768  H6    C A  24      -0.402 -19.203   3.575  1.00  0.00           H
TER     769        C A  24
ENDMDL
MODEL        2
ATOM      1  O5'   G A   1     -10.937 -10.771   1.038  1.00  0.00           O
ATOM      2  C5'   G A   1     -12.150 -10.309   1.638  1.00  0.00           C
//
```

4.1 Open a multistate PDB file

✔ **TASK**

√ - **Open** a new session of PyMol or **MacPyMol**.
√ - **Load** the **1SY4.pdb** file either from the menu (**File > Open…**) or the line command (**load 1SY4.pdb**)
√ - change the background to white (top menu:
Display > Background > White)

PyMol will read all molecule states, in this example 12. This is also echoed within the text panel together with part of the PDB header. However, only ONE structure will be visible at this point.

```
PyMOL>  load 1SY4.pdb
HEADER    RIBONUCLEIC ACID                          31-MAR-04   1SY4
TITLE     REFINED SOLUTION STRUCTURE OF THE S. CEREVISIAE U6
TITLE    2 INTRAMOLECULAR STEM LOOP (ISL) RNA USING RESIDUAL DIPOLAR
TITLE    3 COUPLINGS (RDCS)
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: U6 INTRAMOLECULAR STEM-LOOP RNA;
COMPND   3 CHAIN: A;
COMPND   4 ENGINEERED: YES;
COMPND   5 MUTATION: YES;
COMPND   6 OTHER_DETAILS: MUTATION A62G
 ObjectMolecule: Read crystal symmetry information.
 Symmetry: Found 1 symmetry operators.
 ObjectMolReadPDBStr: read MODEL 1
 ObjectMolReadPDBStr: read MODEL 2
 ObjectMolReadPDBStr: read MODEL 3
 ObjectMolReadPDBStr: read MODEL 4
 ObjectMolReadPDBStr: read MODEL 5
 ObjectMolReadPDBStr: read MODEL 6
 ObjectMolReadPDBStr: read MODEL 7
 ObjectMolReadPDBStr: read MODEL 8
 ObjectMolReadPDBStr: read MODEL 9
 ObjectMolReadPDBStr: read MODEL 10
 ObjectMolReadPDBStr: read MODEL 11
 ObjectMolReadPDBStr: read MODEL 12
 CmdLoad: "1SY4.pdb" loaded as "1SY4".
```

4.2 Dynamic movie:

The 12 structures/models/states can be seen in rapid succession by clicking the play (triangle) and pause (square) buttons on the vcr control at the bottom right.

✔ TASK

√ - **Click** on the **play** () and **pause** () buttons of the vcr control and **observe** the molecule movements between the solved states.

All structures are shown as the default representation (lines). Any changes (e.g. change to sticks) would apply equally to all 12 structures:

√ - Within the **Names Panel** follow the menu cascade: **1SY4 > S > stick**

This animation can be saved as a QuickTime movie as seen previously:

√ - Follow the menu **File > Save Movie As…** menu option to save the movie.
√ - You can change the default name from pymol.mov to **nmr.mov** for example.

4.3 Seprating the models:

Within PyMol each model is called a "state." All models can be extracted as individual objects with a single command: split_states.

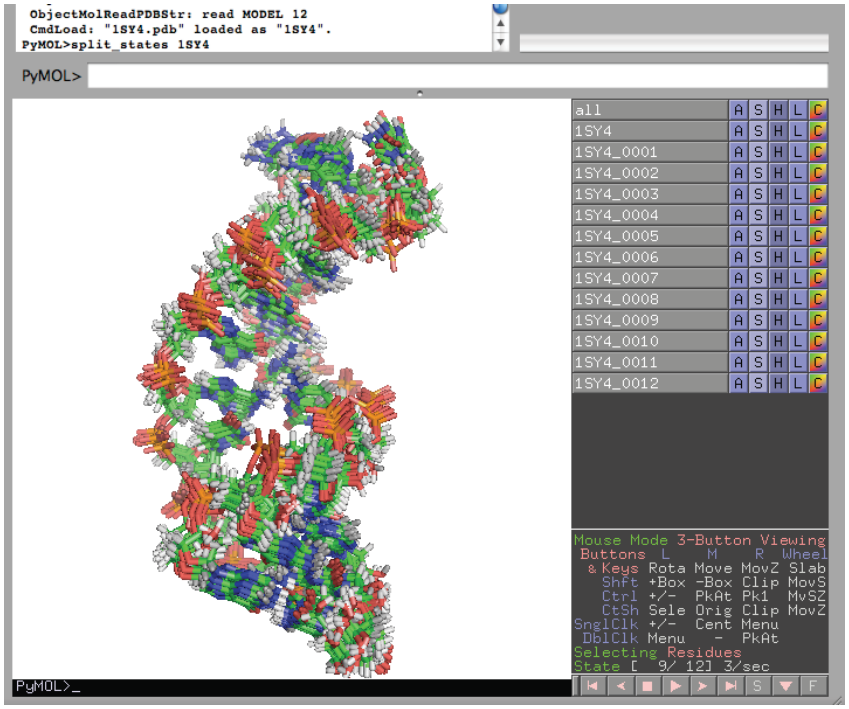
✔ TASK

√ - separate all the states with the line command: **`split_states 1SY4`**

This line-command will separate all the structures and make each one of them a separate object assuming the name of the object is 1SY4.

When the command is given, 12 new objects are created, labeled from 1SY4_0001 to 1SY4_0012.

These can be worked on individually with the help of the ASHLC menus within the Names Panel or made invisible by simply clicking on its name in the Names Panel.



Since all the models are now visible at the same time, the play button on the vcr control has no apparent effect.

Note: the original, single object named 1SY4 containing all 12 structures is still loaded. It could be removed with the action menu cascade: **1SY4 > A > delete object**