

# Guidelines for crafting an effective report

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## 1. Citing Research Articles/publications

We do not impose a specific format for citing publications, we only appreciate consistency: if you start with a format, make sure you use this format consistently.

You will find below information about the 3 main formats that are used for citing papers, namely Vancouver style, APA style, and MLA style.

However, if you are familiar with another format (from other classes for example), do not hesitate to use it.

### **Vancouver style (most popular):**

#### **In-Text Citations:**

- Place a superscript number at the end of the sentence or phrase where you've used information from a source. For example: [HYP is present in Collagen.<sup>1</sup>](#)
- Number the citations consecutively throughout the document.

#### **Reference List:**

- Create a numbered reference list at the end of your document, listing sources in the order they were cited.
- Include details such as author names, title of the work, publication information, etc.

### **APA Style:**

#### **In-Text Citations:**

- When paraphrasing or directly quoting a source within your text, include the author's last name and the publication year in parentheses. For example: [\(AuthorLastName, Year\)](#).
- If the source has multiple authors, use an ampersand (&) between the last names of the authors. For example: [\(Author1LastName & Author2LastName, Year\)](#).
- If the source has more than six authors, use "**et al.**" after the first author's name.

#### **Reference List:**

- At the end of your article, create a separate section titled "References."
- List all the sources you cited in your article in alphabetical order by the author's last name.
- Include the author's name, publication date, title of the work, and publication information.

### MLA Style:

#### In-Text Citations:

- When paraphrasing or directly quoting a source within your text, include the author's last name and the page number in parentheses. For example:  
(AuthorLastName PageNumber).
- If the source has multiple authors, use "et al." after the first author's name.

#### Works Cited:

- At the end of your article, create a separate section titled "Works Cited."
- List all the sources you cited in your article in the order by the author's last name.
- Include the author's name, title of the work, publication information, and other relevant details.

## 2. Citing web sources:

### APA Style:

#### Reference List:

- Author last name, Initials. (Year, Month Day). *Page title*. Website Name. URL

### MLA Style:

#### Works Cited:

- Author last name, First name. "Page Title." *Website Name*, Day Month Year, URL.

#### In-text citations

- Numbering preferred!!!

Keep in mind:

An overly lengthy URL could possibly suggest that a keyword search is intertwined.

Else, it could also suggest that the link you are citing is a research article, in which you should adhere to the rules of section 1 above.

For instance: [https://www.science.org/doi/10.1126/science.7695699?url\\_ver=Z39.88-2003&rfr\\_id=ori:rid:crossref.org&rfr\\_dat=cr\\_pub%20%20pubmed](https://www.science.org/doi/10.1126/science.7695699?url_ver=Z39.88-2003&rfr_id=ori:rid:crossref.org&rfr_dat=cr_pub%20%20pubmed)

Is referring to a science paper and not a web link!

More on: <https://www.scribbr.com/citing-sources/cite-a-website/>

## 3. Saving a script in PyMOL compatible format

The core of PyMOL is written in C, whilst the scripting interface and many extensions are implemented using Python. Therefore, like all other scripting languages PyMOL does not take into account **any** file extension other than its own **.pml extension** or python **.py extension**.

To save a script in a PyMOL compatible extension, type the following code on the console:

“log\_open <space> /path/to/file/scriptname.pml” or  
“log\_open<space>/path/to/file/scriptname.py”

/path/to/file = path where you want the file saved

For example: MacOS: “log\_open /Users/Brian/ECS\_129/project1.pml”  
Windows: “log\_open C:\Desktop\Brian\ECS\_129\project1.pml”

PyMOL allows saving a **PyMOL session** with specific states, settings, and representations, as a session file (**.pse**) using the **save** command with the ".pse" extension. Session files store a more comprehensive set of information about the PyMOL session compared to simple scripts. But **cannot** store your commands. Therefore, DO NOT use this extension to save scripts.

#### 4. Commenting

Comments are Human readable descriptions placed in a code. The purpose is to detail what each code does. Commenting helps in organizing the code and easily fixing bugs.

Comments can be placed on your code simply by editing the script file in any text editor. Place your comments using “#”

Comments will not be executed by an interpreter or a compiler.

For example:

Here is a script with correctly placed comments.

```
UW PICO 5.09                               New Buffer                               Modified
log_open
# Load the structure from PDB
fetch 1a30
# set the background color to white
bg_color white
hide solvent
# Customize protein appearance
set cartoon_fancy_helices
set cartoon_color, hydrogen
set cartoon_transparency, 0.6
# Orient the protein to set the view
orient chain C
log_close
```

More on commenting: <https://users.cs.utah.edu/~germain/PPS/Topics/commenting.html>

## 5. Formatting Images and attaching figure

An image confers several purposes in a report such as visualizing data, visual representation, supporting evidence, clarification of a complex idea. Therefore, Proper representation of figures is important.

- Use different representations to emphasize the structure details.

For instance, Helices cannot be observed properly by a space filling representation.

Refrain from changing the transparency, opacity when it's a 2D rendering.

An opacity difference is only useful to show the structure in 3D. To allow a viewer to gain a sense of dimension for instance if a certain component is immersed deep within a structure or if on the surface. But if the idea is to show 3 helices, variation on the opacity throughout the structure is not necessary.

More on PyMOL representation: <https://www.compchems.com/pymol-colors-and-basic-customization/>

- To render a publication quality image in PyMOL:

“Line 1: set ray\_trace\_mode, 1

Line 2: ray

Line3: png /path/to/file/example\_1.png, dpi=300”

Missing Line 1 and Line 2 would cause you to generate an image with a license caption in green at the top of your image.

DO NOT attach an image with unnecessary ornaments like this caption on your reports.

- PREFER a light background to a dark background for your images. This is not required, but it makes your images easier to read.

- To change the background of an image in PyMOL:

“bg\_color white”

- Placement of the figure titles/ captions

Figure captions and titles serve in helping readers understand and interpret visual elements.

Figures should be labeled with a number followed by a descriptive caption or title.

Captions should be concise but comprehensive. They should describe the data shown, draw attention to important features contained within the figure, and may sometimes also include interpretations of the data.

More on Figure captions: <https://www.scu.edu/media/offices/provost/writing-center/resources/Tips-Figure-Captions.pdf>

Remember Images are the most important aspect of a scientific writing!!

## 6. Confusion between Beta strands and Beta sheets

A Beta-sheet is a more spacious type of secondary structure formed from two or three beta-strands aligned in parallel or antiparallel. Strands consist of the protein backbone “zigzagging”, typically for four to ten residues and is represented as an arrow in cartoon representation in PyMOL. Single  $\beta$ -strands are not energetically favorable which provokes them to form beta sheets adjoined by H-bonds.

The following is a screenshot of a part of a pdb file that explains about the secondary structure content.

HELIX	1	1	VAL	A	29	GLY	A	42	1									14
HELIX	2	2	THR	A	119	ASP	A	123	5									5
HELIX	3	3	GLY	A	135	ARG	A	144	1									10
SHEET	1	AA	8	PHE	A	53	ILE	A	57	0								
SHEET	2	AA	8	MET	A	61	GLY	A	64	-1	0	MET	A	61	N	ILE	A	57
SHEET	3	AA	8	PHE	A	112	CYS	A	115	-1	0	PHE	A	112	N	GLY	A	64
SHEET	4	AA	8	ILE	A	97	MET	A	100	-1	0	ILE	A	97	N	CYS	A	115
SHEET	5	AA	8	VAL	A	128	GLU	A	134	-1	N	PHE	A	129	O	LEU	A	98
SHEET	6	AA	8	GLU	A	15	LEU	A	24	-1	0	SER	A	21	N	LYS	A	133
SHEET	7	AA	8	THR	A	5	VAL	A	12	-1	0	VAL	A	6	N	PHE	A	22
SHEET	8	AA	8	ILE	A	156	GLN	A	163	-1	0	THR	A	157	N	ALA	A	11

But don't be fooled!!

**SHEET** indicates the location, sense (anti-parallel, *etc.*) and registration with respect to the previous strand in the sheet (if any) of each strand in the model. **One record per strand.**

Source: <https://www.cgl.ucsf.edu/chimera/docs/UsersGuide/tutorials/pdbintro.html>

## 7. Think!!

Amino acid contains backbone atoms (C $\alpha$  + NH $_2$  + COOH) + side chain. Backbone atoms bind together by peptide bonds to form polypeptides/proteins. Whereas sidechains are flexible and sticks out of the protein backbone. sidechains give the amino acids certain properties (varying degrees of hydrophobicity, charge, bulkiness, polarity, flexibility) which in turn is translated to the protein. Prolines are unique in that its sidechain connects to the backbone twice. So, what is particularly important about it? Less flexibility. Presence of Proline or Glycine (no sidechain) in a protein makes it stable. Also, if u think about it, any modification to these proteins would directly influence the backbone. Which is why the presence of HYP stabilizes collagen extensively instead of any other polar amino acid like Threonine or Serine (which still can make Hydrogen bonds) substituting in place of HYP!!