



PROTEOPEDIA
—LIFE IN 3D—

A powerful tool for biomolecular
communication
and a 3D encyclopedia of biomolecules

Joel L. Sussman, Eran Hodis & Jaime Prilusky
Weizmann Institute of Science

Visit Proteopedia's main page: <http://proteopedia.org>

1

Let's explore!



Hands-on:

1. Go to <http://proteopedia.org> and type 'Hemoglobin' in the empty white search box on the left-hand toolbar, then press 'Go'.
2. Explore the first section. Stop before 'Hemoglobin subunit binding O2'

2

Let's explore!



Hands-on:

1. Now type 'Peptide' in the empty white search box on the left hand toolbar and press 'Go'. Explore this page.

3

Let's explore!



Hands-on:

1. Navigate back to the 'Main Page' by clicking the link 'Main Page' on the left-hand toolbar.
2. Scroll down to 'What can Proteopedia do for me' and in the 'Educators' column, click on the link 'tutorials or molecular scenes', you will be taken to a new page.
3. Now click on the link titled 'Structural_Templates'
4. Scroll down to the section titled 'Secondary structure elements'.
5. Explore this section, but stop before the section titled 'Turns and loops'

4

STOP (PAUSE) HERE



5

WHAT ARE WE GOING TO LEARN?

- How to create your own pages in Proteopedia, including 3D structures and green scene links.

6

HOW TO EDIT A PAGE (1)

Hands-on:

1. Go to <http://proteopedia.org>
2. Use the search box to get to your assigned Sandbox page.
3. You will need to log in to edit the page. **Log in with a student account given by the instructor.**
4. On your assigned Sandbox page, click on "edit this page".
5. Then scroll down and click the "save page" button. This will 'create' and save your Sandbox page for further editing..

7

HOW TO EDIT A PAGE (2)

- Your page should now look like this:

article | discussion | edit this page | history | move | watch | log out

Sandbox 759

Your Heading Here (maybe something like 'Structure') [edit]

Anything in this section will appear adjacent to the 3D structure and will be scrollable.

toggle spin | toggle quality | popup

Jmol

Scrollable section

Structure of HMG-CoA reductase (PDB entry 1dq8)

8

HOW TO EDIT A PAGE (3)

Hands-on:

1. Open a new browser window and navigate to the page "Sandbox" (with no additional number) in Proteopedia.
2. Click on the link to reach an example page on Green Fluorescent Protein. We will recreate this page in Proteopedia as an example. [http://proteopedia.org/wiki/index.php/User:Joel L. Sussman/GFP Test Page](http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page) -- keep this page open throughout the workshop.
3. Select the two paragraphs of text, and copy them (ctrl-v). Start from "Green Fluorescent Protein..." and include the heading "Exploring the Structure" as well as both paragraphs.
4. Go back to the browser window with your assigned Sandbox page (the one you cleared earlier), and click "edit this page".
5. Some automatic text appears in the text-editing area. This text is meant to help you get started editing, but we don't need it now. Delete it.
6. In the now-blank text-editing area, paste the text that you copied in step (3). Save using the "Save page" button.

9

HOW TO EDIT A PAGE (4)

- Your page should now look like this:

Joel L. Sussman my talk my preferences my watchlist my contributions log out
article discussion **edit this page** history protect delete move

Sandbox 759

Green fluorescent protein (GFP), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The chromophore, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues.

10

ADDING SECTION HEADINGS

Hands-on:

1. In your assigned Sandbox page, now displaying your new text, click "edit this page".
2. We want to make "Exploring the Structure" as a section heading. Highlight the text "Exploring the Structure" and select the button from the toolbar above the text-editing area with a big "A".
3. The result should be two equals signs on either side of the words "Exploring the Structure". It should look like this: ==Exploring the Structure==.
4. Save the page using the "Save page" button.



11

ADDING SECTION HEADINGS

- Your page should now look like this:

Joel L. Sussman my talk my preferences my watchlist my contributions log out
article discussion **edit this page** history protect delete move

Sandbox 759

Green fluorescent protein (GFP), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

==Exploring the Structure== [edit]

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The chromophore, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues.

12

BOLD AND INTERWIKI LINKS

Hands-on:

1. In your assigned Sandbox page, now displaying your new text, click "edit this page".
2. We want to make the word "GFP" bold. Select the word "GFP" and click on the button in the toolbar above the text-editing area with a big "B".
3. The result should be three single quotation marks on either side of the word "GFP" like so: "'GFP'"
4. Now make "1ema" into an interwiki link, so that it leads to the Proteopedia page for the PDB entry 1ema. Do this by selecting the text "1ema" and clicking on the button in the toolbar above the text-editing area with a big, underlined, blue "Ab".
5. The result should be two square inward-facing brackets on either side of the word "1ema". It should look like this: `[[1ema]]`
6. Save the page using the "Save page" button.



13

BOLD AND INTERWIKI LINKS

- Your page should now look like this:

Joel L. Sussman my talk my preferences my watchlist my contributions log out
article discussion edit this page history protect delete move

Sandbox 759

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry **1ema**), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure [edit]

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The chromophore, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine

14

ADDING A 3D STRUCTURE (1)

Hands-on:

1. We'd now like to add a 3D structure to the page (by adding a Jmol applet displaying the 3D structure for PDB entry 1ema, the structure of Green Fluorescent Protein).
2. In your assigned Sandbox page click on "edit this page".
3. In the text-editing area, click on the top of the page, so that the cursor is blinking on a new line before all your text.
4. In the toolbar above the text-editing area, click on the **green squares** button .
5. In the new text that appears, replace the text
 1. "Anything in this section will appear adjacent . . . and will be scrollable." with the two paragraphs of text you previously copied.
 2. load='1dq8' with "load='1ema'"
 3. caption='Structure of HMG-CoA reductase (PDB entry [[1dq8]]) with caption='GFP (PDB entry [[1ema]])
6. The newly added text should now begin like: "==Your Heading Here (maybe something like 'Structure')==
Preview the page using the "Preview page" button. (Not "Save"!)



15

Your page should now look like this:

Joel L. Sussman my talk my preferences my watchlist m
article discussion edit this page history protect delete move watch

Editing Sandbox 759

Preview

This is only a preview; changes have not yet been saved!

==Your Heading Here (maybe something like 'Structure')==

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry **1ema**), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The chromophore, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central

16

ADDING A 3D STRUCTURE (2)

Hands-on:

1. "Preview page" lets us see how the page will look, without saving it.
2. In our Preview, we see that the 3D Jmol applet displaying our structure is a bit too large,
3. So, scroll down to the text-editing area (notice that the "Preview" contains the text-editing area on the page).
4. Replace, in the top line of text:
 1. "size='500'" with "size='300'"
5. Save the page using the "Save page" button.

==Your Heading Here (maybe something like 'Structure')==<StructureSection load='1ema' size='500' side='right' caption='GFP (PDB entry [[1ema]])' scene='>Green fluorescent protein ("GFP"), originally isolated from the jellyfish Aequorea victoria (PDB entry [[1ema]]), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is

17

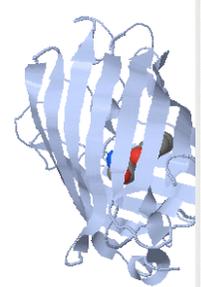
Joel L. Sussman my talk my preferences my watchlist my cont

article discussion edit this page history protect delete m

Sandbox 759

==Your Heading Here (maybe something like 'Structure')==

Green fluorescent protein (GFP), originally isolated from the jellyfish Aequorea victoria (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.



toggle spin toggle quality popup

GFP (PDB entry 1ema)

Proteopedia - Life in 3D

navigation

- Main Page
- Table of Contents
- Structure Index
- Random
- Recent Changes
- Help

search

Go Search

Google Custom Search

Google Search

toolbox

- What links here
- Related changes
- Upload file
- Special pages
- Printable version

Your page should now look like this:

18

ADDING A GREEN SCENE LINK (1)

Hands-on:

1. Now that we have a 3D model on the page, let's create a **green scene link** that shows 1ema as it looks in the the left part of the 2D image on the GFP Sample page where we got our text. (go back to that page to see what the picture looks like: ([http://proteopedia.org/wiki/index.php/User:Joel L. Sussman/GFP Test Page](http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page)))
2. To create a green scene link, we will need to use the *Proteopedia Scene Authoring Tools*.
3. In your assigned Sandbox page, click on "edit this page".
4. Scroll down to the bold text that says "Scene authoring tools [show]" next to a colorful molecule. Click on "show" to expand the Scene Authoring Tools.
5. Click on the tab "load molecule" in the Scene Authoring Tools.
6. Load the PDB file 1ema by entering the PDB code "1ema" in the input box next to the words "By PDB code:" and then pressing the adjacent button marked "load".

19

Scene authoring tools [hide]

how to load scene save scene load molecule selections representations colors labels

load molecule

By PDB code: 1ema load

From Proteopedia uploaded file: load

To load from an uploaded file, first upload the file to Proteopedia.



Jmol S

currently loaded file	source	timestamp
1ema	PDB	20090520

select all select none popup

< undo redo >

selection halos:

To enable buttons below, save your scene, if desired, then hide the Scene Authoring Tools.

Summary:

Your page should now look like this:

20

ADDING A GREEN SCENE LINK (2)

Hands-on:

1. Now we have 1ema loaded into the Scene Authoring Tools' Jmol applet. The idea behind the Scene Authoring Tools (SAT) is to create the exact scene that you would like to have load when your **green link** is clicked. This is generally done by first loading a PDB file into the SAT's applet, then using the "selections", "representations", "colors", and "labels" tabs to manipulate the 3D model into the desired state, finally saving the **green scene link** using the "save scene" tab.
2. Our structure is currently displayed in cartoon representation. The first step in recreating the picture in the *Molecule of the Month* is to display the molecule in backbone representation.
3. Click on the "selections" tab.
4. In the "all or nothing and halos" section, click on the "select all" button.
5. Nothing changed because "selection halos" were not on. Turn them on by marking the checkbox next to the word "selection halos".
6. Selection halos serve to show you what is currently selected. They will not be displayed when the **green scene link** you eventually create is clicked.

21

Your page should now look like this:

how to | load scene | save scene | load molecule | **selections** | representations | colors | labels

build your selection

groups: all protein alpha carbon backbone/mainchain helix sheet sidechain turn non-protein

limit to chains: all limit to residue types: all

e.g. A,C,D e.g. PHE,ALA,GLY

limit to residue numbers: all

e.g. 18,29-25,32

limit to elements: all

e.g. Fe,2H,3IP

Hold ctrl to select multiple groups

replace selection | add to selection | remove from selection

invert and center

invert current selection | center on current selection

select within distance

Select atoms within Å of current selection. go

Expand selection to include entire residues containing any selected atoms. go

mouse click selects

nothing center atom element residue/ligand chain

Jmol_S

currently loaded file source timestamp

1ema PDB 20090520

select all | select none | popup

< undo | redo >

selection halos:

22

ADDING A GREEN SCENE LINK (3)

Hands-on:

1. Now that we have everything selected, click on the "representations" tab of the SAT.
2. Mark the checkbox next to "backbone" in the section titled "set selection representation".
3. Click on the "set representation" button.
4. Notice the representation of the 3D model has changed from cartoon to backbone. To help see this better, turn off the selection halos by unmarking the checkbox next to "selection halos".

23

Your page should now look like this:

how to | load scene | save scene | load molecule | selections | **representations** | colors | labels

set selection representation

ball and stick stick/wireframe 90

spacefill 100% dots 100% backbone 90

trace 90 ribbon cartoon

strands rocket meshribbon 2.5

surface halos

Leaving the input field to the right of a representation-type blank chooses its default setting.
Ball and stick is a combination of wireframe and spacefill.

set representation

hide selection

disulfide and hydrogen bonds [show]

Jmol_S

currently loaded file source timestamp

1ema PDB 20090520

select all | select none | popup

< undo | redo >

selection halos:

24

ADDING A GREEN SCENE LINK (4)

Hands-on:

1. Now we want to select the segment of the protein that runs through the barrel and color it green.
2. To make a selection, click on the "selections" tab.
3. We will select the segment that runs through the barrel by its residue numbers. To do this we need to know the first and the last residue numbers that make up this segment.
4. Notice that when you hover with your mouse over an atom in the Jmol applet, information about that atom is displayed, including the residue that atom is part of, and the residue number. Use this "hover" feature to find the residue numbers for the beginning and the end of the segment we are interested in.
5. Enter the starting and ending residue numbers, separated by a hyphen, into the input box under the text "limit to residue numbers:".

25

Your page should now look like this:

how to | load scene | save scene | load molecule | **selections** | representations | colors | labels

build your selection

groups: **non-protein**
Hold ctrl to select multiple groups

limit to chains: e.g. A,C,D

limit to residue types: e.g. PHE,ALA,GLY

limit to residue numbers: e.g. 18,23-25,32

limit to elements: e.g. Fe,2H,31P

replace selection | add to selection | remove from selection

invert and center
invert current selection | center on current selection

select within distance
Select atoms within Å of current selection.
Expand selection to include entire residues containing any selected atoms.

currently loaded file: 1ema source: PDB timestamp: 20090520

select all | select none | popup
< undo | redo >
selection halos:

26

ADDING A GREEN SCENE LINK (5)

Hands-on:

1. Having entered the starting and ending residue numbers of the chain segment into the "limit by residue numbers" input box, we are ready to make a selection that is limited only to the stretch of residues that we desire.
2. Before making our new selection, let's turn on selection halos so we see the change in the selection take place. Mark the checkbox next to "selection halos". Notice that everything is selected.
3. Now go ahead and make the new selection by clicking "replace selection". This will replace the old selection (everything) with our new selection (limited to a stretch of residues).

27

Your page should now look like this:

how to | load scene | save scene | load molecule | **selections** | representations | colors | labels

build your selection

groups: **non-protein**
Hold ctrl to select multiple groups

limit to chains: e.g. A,C,D

limit to residue types: e.g. PHE,ALA,GLY

limit to residue numbers: e.g. 18,23-25,32

limit to elements: e.g. Fe,2H,31P

replace selection | add to selection | remove from selection

invert and center
invert current selection | center on current selection

select within distance
Select atoms within Å of current selection.
Expand selection to include entire residues containing any selected atoms.

currently loaded file: 1ema source: PDB timestamp: 20090520

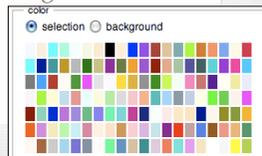
select all | select none | popup
< undo | redo >
selection halos:

28

ADDING A GREEN SCENE LINK (6)

Hands-on:

1. With the chain segment selected, it's time to change its color to match the image in the Molecule of the Month.
2. Click on the "colors" tab of the Scene Authoring Tools.
3. Click on a green color in the color palette to change the color of the selected chain segment. Turn off selection halos to better view the change in color.
4. Now let's make the background black.
5. In the section titled "color", mark the button next to "background". Now any color you select from the color palette will affect the background instead of the selection.
6. Click on the color black in the color palette.



29

Your page should now look like this:

A screenshot of the Jmol interface. The 'colors' tab is selected in the top navigation bar. The 'background' radio button is selected in the 'color' section. The background of the 3D molecular model is black. The 'selection halos' checkbox is unchecked.

30

ADDING A GREEN SCENE LINK (7)

Hands-on:

1. All that's left is to show the chromophore and color it in the CPK scheme.
2. Click on the "selections" tab.
3. In the input box under "limit to residue types:" type "CRO". (In the PDB file, the chromophore is listed as a residue with type "CRO")
4. Click on the "replace selection" button. Turn on selection halos.
5. Click on the "representations" tab.
6. In the section titled "set selection representation" mark the checkbox next to stick/wireframe. Click on the "set representation" button.
7. Click on the "colors" tab.
8. In the section titled "color" click on the button titled "CPK (by element)".
9. Turn off selection halos to better view the new color.

31

Your page should now look like this:

A screenshot of the Jmol interface. The 'colors' tab is selected. The 'CPK (by element)' button is selected in the 'color' section. The chromophore in the 3D model is highlighted in green. The 'selection halos' checkbox is unchecked.

32

ADDING A GREEN SCENE LINK (8)

Hands-on:

1. Notice that connection between the chromophore & the chain is missing, but is seen in the original picture: http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page. Let's visualize those missing bonds in the chain.
2. Click on the "selections" tab; in the 'build your selection' box, under 'groups' select 'backbone/mainchain'; In the input box under "limit to residue numbers:" type "64,68". (These are the numbers of the residues directly preceding and following the chromophore.)
3. Click on the "add to selection" button.
4. Click on the "representations" tab.
5. In the section titled "set selection representation" mark the checkbox next to stick/wireframe. Click on the "set representation" button.
6. Click on the "colors" tab.
7. In the section titled "color" click on the button titled "CPK (by element)".
8. Turn off selection halos to better view the new color.

33

ADDING A GREEN SCENE LINK (9)

Hands-on:

1. Our scene is done, so let's save it and put it into the page.
2. Click on the "save scene" tab in the Scene Authoring Tools.
3. Give your scene a name and a description by entering text in the "Name" and "Description" text-areas.
4. Let's make our scene spin when it loads. In the drop down menu next to the text "when this scene loads, I want it to" choose the option "spin".
5. Click on the "save scene" button.

34

Your page should now look like this:

how to | load scene | **save scene** | load molecule | selections | representations | colors | labels

Save current scene

Scene name
1_ema_chromophore
e.g. Active_site_gorge
Enter an existing scene name to save as the most recent version (will not overwrite).

Scene description (recommended)
GFP (PDF 1ema) with the chromophore shown in the middle of the protein barrel.

when this scene loads, I want it to spin

Always Reload Structure When Loading this Scene

show scene transition options?

Save current scene

Wikitext

Copy and paste the following line where you want the scene link to appear (scroll down if needed) and edit the TextToBeDisplayed:

```
<scene name='56/561617/1_ema_chromophore /1'>TextToBeDisplayed</scene>
```

Upon saving a scene, wikitext for creating a link to the saved scene will appear above.

currently loaded file: 1ema | source: PDB | timestamp: 20090520

select all | select none | popup

< undo > | > redo >

selection halos:

35

ADDING A GREEN SCENE LINK (9)

Hands-on:

1. As soon as we saved our scene, some wikitext appeared in the text-area titled "Wikitext" that was previously empty.
2. The new text in the "Wikitext" text-area instructs you to copy a line in the text-area & paste it in the text of the Proteopedia page where you would like the green scene link to appear. The line looks similar to this: `<scene name='56/561617/1_ema_chromophore/1'>TextToBeDisplayed</scene>`
3. Highlight that line in the "Wikitext" text-area and copy it.
4. Scroll up the page, past the Scene Authoring Tools to the text-editing area of the Proteopedia page.
5. Find the word "chromophore" in the text-editing area. Highlight it and replace it by pasting the text you previously copied in step (3).

36

Your page should now look like this:

Editing Sandbox 759



```
==Your Heading Here (maybe something like 'Structure')==<StructureSection load='1ema' size='300'
side='right' caption='GFP (PDB entry [[1ema]])' scene=''>Green fluorescent protein (''GFP''),
originally isolated from the jellyfish Aequorea victoria (PDB entry [[1ema]]), fluoresces green (509nm)
when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in
biological research because it can be used to tag otherwise invisible gene products of interest and thus
observe their existence, location and movement.
```

```
== Exploring the Structure ==
```

```
GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids.
The <scene name='56/561617/1_ema_chromophore/1'>TextToBeDisplayed</scene> responsible for the
fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha
helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of
three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation
creates the chromophore's five-membered ring via a new bond between the threonine and the glycine
residues.</StructureSection>
```

37

ADDING A GREEN SCENE LINK (10)

Hands-on:

1. The text that you just pasted from the "Wikitext" section of the Scene Authoring Tools creates a **green scene link** wherever you place it in the Proteopedia page.
2. The word "TextToBeDisplayed" will be the part that shows up as the text of the green link on the page.
3. Change "TextToBeDisplayed" to say "chromophore. It should look something like:
<scene name='Sandbox_3/1ema/1'>chromophore</scene>
4. Scroll down to the bold text "Scene Authoring Tools [hide]" next to the colored molecule, and click on "hide" to hide the Scene Authoring Tools.
5. Scroll down and click on "Save page" to save the Proteopedia page you edited.
6. Try clicking on the new **green scene link** you have created.

38

Your page should now look like this:

Joel L. Sussman my talk my preferences my watchlist my contributions log out

article discussion edit this page history protect delete move watch

Sandbox 759

==Your Heading Here (maybe something like 'Structure')==

Green fluorescent protein (GFP), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues.

Scrollable section

toggle spin toggle quality popup

GFP (PDB entry 1ema)

39

ADDING A 'HEADING'

Hands-on:

1. To make the page look nicer, need add a 'Heading' to first paragraph.
2. Go back and Edit your page
3. Change, in the top line of your text
 - ==Your Heading Here (maybe something like 'Structure')==<StructureSection. . .
 - to
 - == Example page for Green fluorescent protein ("GFP") ==<StructureSection. . .
4. Save page

40

Your page should now look like this:

Joel L. Sussman my talk my preferences my watchlist my

article discussion edit this page history protect delete move

Sandbox 759

Example page for Green fluorescent protein ("GFP")

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

toggle spin toggle quality po

GFP (PDB entry 1ema)

navigation

- Main Page
- Table of Contents
- Structure Index
- Random
- Recent Changes
- Help

search

Go Search

Google Custom Search

Google Search

toolbox

- What links here
- Related changes
- Upload file
- Special pages

Scrollable section

41

ADDING A REFERENCE

Hands-on:

- Let's cite a reference in our page. Look at the reference at the bottom of our original example page: http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page.
- We could add the reference by typing it out -- that's the long way.
- A much easier way is to refer to the paper by its PubMed ID: Click on 'edit this page' for your 'Sandbox' page. At the end of the 2nd paragraph, after the words 'the glycine residues', add the text '<ref>PMID:8703075</ref>'.
- '<ref>' is called the opening reference tag, and '</ref>' is the closing tag. Together they enclose the text 'PMID:' which stands for PubMed ID, and then the actual PubMed ID of the reference you want to cite.
- You've added the citation, but you still need to specify where the bibliography will appear -- the list of all cited references in the page.
- Do this by adding the line '<references/>' after the last paragraph. Save the page.

42



navigation

- Main Page
- Table of Contents
- Structure Index
- Random
- Recent Changes
- Help

search

Go Search

Google Custom Search

Google Search

toolbox

- What links here
- Related changes
- Upload file
- Special pages

Joel L. Sussman my talk my preferences my watchlist my contributions log out

article discussion edit this page history protect delete move watch

9 open e-mail-confirmed account requests pending

Editing Sandbox 759

B Ab A

```

=== Example page for Green fluorescent protein ("GFP") ===
<StructureSection load='1ema' size='300' side='right' caption='GFP (PDB entry [[1ema]])' scene=''>Green fluorescent protein (''GFP''), originally isolated from the jellyfish Aequorea victoria (PDB entry ''[[1ema]]''), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

=== Exploring the Structure ===

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The <scene name='56/561617/1_ema_chromophore /1'>chromophore</scene>, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residue <ref>PMID:8703075</ref>.
</StructureSection>

=== References ===
<references/>

```

Please note that all contributions to Proteopedia may be edited, altered, or removed by other contributors. If you

43

Joel L. Sussman my talk my preferences my watchlist my cont

article discussion edit this page history protect delete move watch

Sandbox 759

Example page for Green fluorescent protein ("GFP")

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry 1ema), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

toggle spin toggle quality popup

GFP (PDB entry 1ema)

navigation

- Main Page
- Table of Contents
- Structure Index
- Random
- Recent Changes
- Help

search

Go Search

Google Custom Search

Google Search

toolbox

- What links here
- Related changes
- Upload file
- Special pages
- Printable version
- Permanent link

Scrollable section

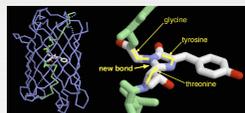
References

- Ormo M, Cubitt AB, Kallio K, Gross LA, Tsien RY, Remington SJ. Crystal structure of the *Aequorea victoria* fluorescent protein. *Science*. 1996 Sep 6;273(5280):1392-5. PMID:8703075

Your page should now look like this:

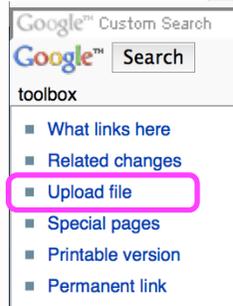
44

ADDING A 2D IMAGE (1)



Hands-on:

- Let's add a 2D image to our page. View our example page http://proteopedia.org/wiki/index.php/User:Joel_L._Sussman/GFP_Test_Page and save the big picture to your computer by right-clicking on it and choosing an option like "Save as..." or "Save to desktop". Save the image (1ema.gif) to your desktop.
- We now need to upload the image to Proteopedia. Back in your Proteopedia 'Sandbox' page, click on the 'upload file' link in the left-hand toolbar



45

ADDING A 2D IMAGE (2)

Hands-on:

- At the 'upload file' page, next to 'Source filename:' click on the 'Choose file' button. Using the interface that pops up, browse to and select the 2D image we saved (1ema.gif). **Choose File**
- On the 'upload file' page, make sure to change the 'Destination filename' from '1ema.gif' to something unique like '1ema_Workshop_579.gif' where 'Workshop' is the name of your workshop, and '579' is your 'Sandbox' number.
- Under 'Summary' type a short summary of what we see in the picture 1ema.gif.
- Click on the 'Upload file' button. **Upload file**
- Your file will be uploaded and you will be taken to its new page in Proteopedia.
- Copy the image's name, so you have it for later:



46

ADDING A 2D IMAGE (3)

Hands-on:

- Go back to your 'Sandbox' page and click on 'edit this page'.
- Click on the text-editing area just before text "Green fluorescent protein . . ." and hit carriage return to add one blank line.
- Click so that your cursor is in the white space you just created.
- Now click on the button that looks like a picture. This will insert wiki-text for a 2D image.

Editing Sandbox 759



```
== Example page for Green fluorescent protein ("GFP") ==  
<StructureSection load='1ema' size='300' side='right' caption='G:  
(PDB entry [[1ema]])' scene=''>
```

| <--- Cursor here

Green fluorescent protein (''GFP''), originally isolated from

47

ADDING A 2D IMAGE (4)

Hands-on:

- After you clicked on the button that looks like a picture, some wiki-text should have popped up that says '[[Image:Example.jpg]]'.
- Note that this format of double square brackets is the same format as for internal links that we created earlier to '1ema' ([[1ema]]).
- Change the word 'Example.jpg' to the name of your image (remember, you copied the name of your image before, now it comes in handy, you may paste it.)
- The final result should look something like this '[[Image:1ema_Workshop_579.jpg]]'
- Save the page.



```
<StructureSection load='1ema' size='300' side='right'  
caption='GFP (PDB entry [[1ema]])' scene=''>
```

[[Image:1ema.gif]]

Green fluorescent protein (''GFP''), originally iso:
the jellyfish *Aequorea victoria* (PDB entry [[1ema]]),

48

ADDING A 2D IMAGE (5)

Hands-on:

1. At this point you should see the 2D image on your page, but it should be huge -- way too big for us. Let's change that -- click on 'edit this page'
2. Change '[[Image:1ema.gif]]' by adding additional parameters, each separated by a vertical bar '|'.
3. You should change it to read:
'[[Image:1ema.gif|thumb|left|350px|Green fluorescent protein (1ema)]]'
4. This specifies that the image should be a thumbnail on the left side of the page of size 350 pixels and with the caption 'Green fluorescent protein (1ema)'.
5. Save the page.



```
(PDB entry [[1ema]])' scene=''>
```

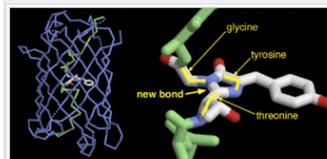
```
[[Image:1ema.gif|thumb|left|350px|Green fluorescent protein (1ema)]]  
Green fluorescent protein ( "GFP" ), originally isolated from the
```

49

Your page should now look like this:

Sandbox 759

Example page for Green fluorescent protein ("GFP")



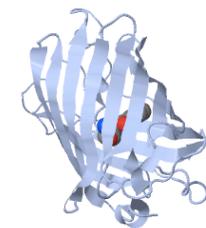
Green fluorescent protein (1ema)

Green fluorescent protein (**GFP**), originally isolated from the jellyfish *Aequorea victoria* (PDB entry [1ema](#)), fluoresces green (509nm) when exposed to blue light (395nm and 475nm). It is one of the most important proteins used in biological research because it can be used to tag otherwise invisible gene products of interest and thus observe their existence, location and movement.

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues¹.

Scrollable section



Jmol

toggle spin toggle quality popup

GFP (PDB entry [1ema](#))

References

1. Ormo M, Cubitt AB, Kallio K, Gross LA, Tsien RY, Remington SJ. Crystal structure of the *Aequorea victoria* green fluorescent protein. *Science*. 1996 Sep 6;273(5280):1392-5. PMID:8703075

50

ADDING A QUIZ

Hands-on:

1. We want to add a quiz to the page to test the reader's comprehension. Click on 'edit this page'.
2. Add the following text after the line '<references/>'.
3. '==Quiz==' is a section heading as before. The rest is wiki-text for a quiz. Save page.

The question is between two curly brackets. Each potential answer is on its own line. A wrong answer is preceded by a minus ('-') sign and the correct answer by the plus ('+') sign.

```
<references/>
```

```
==Quiz==  
<quiz display=simple>  
{How many alpha helices are in this structure?}  
- One  
- None  
+ Eleven  
- Twelve  
</quiz>
```

Please note that all contributions to Proteopedia

51

Your page should now look like this:

Exploring the Structure

GFP is a beta barrel protein with 11 beta sheets. It is a 26.9kDa protein made up of 238 amino acids. The **chromophore**, responsible for the fluorescent properties of the protein, is buried inside the beta barrel as part of the central alpha helix passing through the barrel. The chromophore forms via spontaneous cyclization and oxidation of three residues in the central alpha helix: -Thr65 (or Ser65)-Tyr66-Gly67. This cyclization and oxidation creates the chromophore's five-membered ring via a new bond between the threonine and the glycine residues¹.

Scrollable section



toggle spin toggle quality popup

GFP (PDB entry [1ema](#))

References

1. Ormo M, Cubitt AB, Kallio K, Gross LA, Tsien RY, Remington SJ. Crystal structure of the *Aequorea victoria* green fluorescent protein. *Science*. 1996 Sep 6;273(5280):1392-5. PMID:8703075

Quiz

Points added for a correct answer:

Points for a wrong answer:

Ignore the questions' coefficients:

[Shuffle questions](#)

1. How many alpha helices are in this structure?

- One
 None
 Eleven
 Twelve

-Try taking your quiz by selecting an answer and clicking on the 'Submit' button.-

52

YOUR OWN ACCOUNT

- If you want to use Proteopedia in the future to create your own pages, please request your own account in your own name. You can do this now if you want!
- Request an account in your name by logging out of guest account and clicking “log in / request account” at top right corner of website. Enter the information that is requested, and your account will be approved by Prof. Eric Martz (Univ of Mass).

53

HELP RESOURCES



- General Help: <http://www.proteopedia.org/wiki/index.php/Help:Contents>
- Editing Help: <http://www.proteopedia.org/wiki/index.php/Help:Editing>
- Wikitext Cheatsheet: <http://en.wikipedia.org/wiki/Wikipedia:Cheatsheet>
- Scene Authoring Tools Help: http://www.proteopedia.org/wiki/index.php/Scene_authoring_tools
- Proteopedia Video Guide: http://www.proteopedia.org/wiki/index.php/Proteopedia:Video_Guide

54

GREAT PROTEOPEDIA PAGE EXAMPLES TO EXPLORE

- Lac Repressor :
http://www.proteopedia.org/w/Lac_repressor
- 2q66 - Poly(A) polymerase :
<http://www.proteopedia.org/w/2q66>
- HIV-1 Protease :
http://www.proteopedia.org/w/HIV-1_protease
- Avian Influenza Neuraminidase, Tamiflu and Relenza :
http://www.proteopedia.org/w/Avian_Influenza_Neuraminidase%2C_Tamiflu_and_Relenza
- Recoverin: a calcium-activated myristoyl switch :
http://www.proteopedia.org/w/Recoverin%2C_a_calcium-activated_myristoyl_switch
- [A Physical Model of the \$\beta\$ 2-Adrenergic Receptor](http://proteopedia.org/w/Group:SMART:A_Physical_Model_of_the_%CE%B2-Adrenergic_Receptor)
http://proteopedia.org/w/Group:SMART:A_Physical_Model_of_the_%CE%B2-Adrenergic_Receptor



55

References:



- Hodis, Prilusky, Martz, Silman, Moulton & Sussman (2008) “Proteopedia – a scientific ‘wiki’ bridging the rift between 3D structure and function of biomacromolecules” *Genome Biol* **9**, R121.
- Prilusky, Hodis, Canner, Decatur, Oberholser, Martz, Berchanski, Harel & Sussman (2011) “Proteopedia: A status report on the collaborative, 3D web-encyclopedia of proteins and other biomolecules” *J of Struct Biol* **175**, 244-252.
- Hanson, Prilusky, Renjian, Nakane & Sussman (2013) “JSmol and the Next-Generation Web-Based Representation of 3D Molecular Structure as Applied to Proteopedia” *Israel J of Chem* **53**, 207-216.

56