

TOOLS TO MAKE 3D STRUCTURAL DATA MORE COMPREHENSIBLE: EMOVIE & PROTEOPEDIA

ERAN HODIS^{1,2}, JAIME PRILUSKY^{2,3},
JOEL L. SUSSMAN^{1,2*}

¹*Department of Structural Biology, Weizmann Institute
of Science, Rehovot, Israel*

²*The Israel Structural Proteomics Center, Weizmann Institute
of Science, Rehovot, Israel*

³*Biological Services Unit, Weizmann Institute of Science,
Rehovot, Israel*

Abstract. To the crystallographer, solving a three-dimensional (3D) protein or molecular structure often times feels like the ultimate success, and surely it is. However, of utmost importance is the communication of the insights revealed by the 3D structure, especially those insights that relate structure to function. In order for these insights to reach their potential for guiding future research, they must reach biologists. The problem is that 3D structures are inherently complex and thus communicating insights about 3D structures to non-structural biologists can be difficult. To aid the structural biologist in this endeavor, we have created two useful tools. The first, *eMovie*, is a plug-in for PyMOL that makes creating macromolecular animations much more simple. The second, *Proteopedia*, is a community-annotated ‘wiki’ web-resource that links descriptive text to 3D views of structures, resulting in intuitive communication of structural information.

Keywords: Communicating structural biology, 3D, animations, movies, dissemination, wiki, eMovie, Proteopedia, education, instruction

* To whom correspondence should be addressed. Joel L. Sussman, Department of Structural Biology, Weizmann Institute of Science, Rehovot 76100, Israel; e-mail: Joel.Sussman@weizmann.ac.il

1. Introduction

We present here two tools to aid in the communication of structural biology. One is a tool called eMovie¹ that facilitates the creation of molecular animations. The other is a large-scope, ‘wiki’ web resource called Proteopedia² that has a powerful capability for communicating three-dimensional (3D) structures by linking descriptive text to 3D views of the structure.

They are disparate tools, and thus we present them in separate sections, but it should be noted that movies created using eMovie can be uploaded to Proteopedia to aid in the description of a particular protein, molecule, or concept.

2. eMovie

2.1. ABSTRACT

The 3D structures of macromolecules are difficult to grasp and also to communicate. By their nature, movies or animations are particularly useful for highlighting key features by offering a ‘guided tour’ of structures and conformation changes. However, high-quality movies are rarely seen because they are currently difficult and time consuming to make. By adopting the traditional movie ‘storyboard’ concept, which gives guidance and direction to filming, eMovie makes the creation of lengthy molecular animations much easier. This tool is a plug-in for the open-source molecular graphics program PyMOL, and enables experts and novices alike to produce informative and high-quality molecular animations.

2.2. INTRODUCTION

Soon after the first 3D structures of biological macromolecules were determined, it became clear that visualization and comparison of these structures is crucial to understand their structure and function. The field of molecular graphics was pioneered by Cyrus Levinthal in the 1960s,³ the ‘3D effect’ being achieved by rotating the macromolecular structure constantly on the screen, like a ‘real-time’ movie. The largest drawback was that the computer system – a specialized and extremely large Digital Equipment Computer dedicated to this task, nicknamed the ‘Kluge’ – cost well over US\$300,000. However, during the past 40 years, both hardware and software have progressed enormously (<http://www.umass.edu/microbio/rasmol/history.htm>) making it possible to accomplish much more on a standard desktop computer than was ever possible using the Kluge. A few notable examples of molecular visualization programs that have taken advantage of the improved

technology include Kinemage,⁴ the RasMol-based⁵ 3DBrowser^{6,7} and Protein Explorer (<http://www.umass.edu/microbio/chime/explorer>) and the Jmol-based (<http://www.jmol.org>) FirstGlance in Jmol (<http://molvis.sdsc.edu/fгий>).

Here, we present ‘eMovie’ – a tool for making the process of molecular movie creation more fluid and natural. It is more similar to traditional movie-editing programs and can be used to create extended, complex animations. eMovie introduces a storyboard to the world of molecular animation in addition to modular, insertable actions. Thus, the user can focus on the scientific story rather than the technicalities of animation.

eMovie has been created as a plug-in for the molecular display program PyMOL. PyMOL combines superior picture quality with a highly advanced scripting interface, including versatile animation commands that can create long, complex movies; however, accessing the animation commands through the command line is difficult and error-prone. A new user is faced with a steep learning curve given the complicated animation commands and the necessity for writing external scripts. eMovie resolves these issues by providing a simple graphical interface through which the user can interact with the powerful movie-making capabilities of PyMOL without needing familiarity with commands, syntax or external scripts.

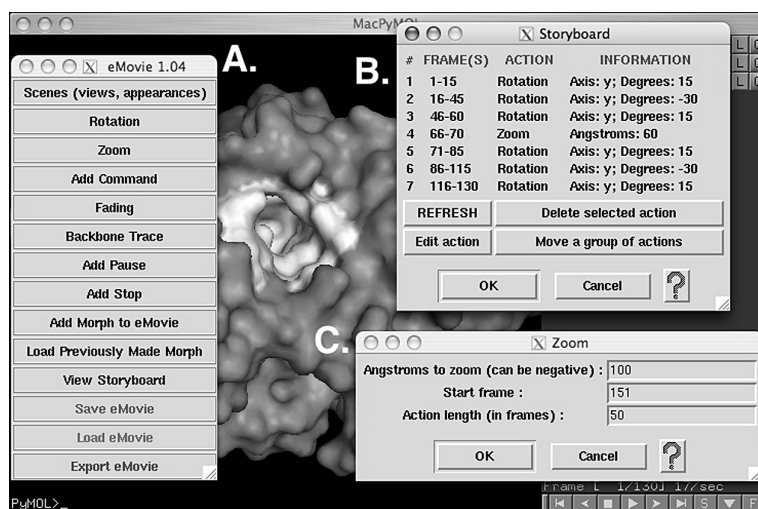


Figure 1. Snapshot of eMovie in action. In the background is the PyMOL GUI and the eMovie plug-in, with three open windows appears in the foreground. (A) The eMovie main menu bar with all of the buttons for inserting modular actions and viewing the storyboard (B) The storyboard window has been opened as a result of clicking “View Storyboard” on the eMovie menu bar. The storyboard displays the modular actions comprising the movie and invites the user to make changes. (C) The zoom window has been opened as a result of clicking “Zoom”. A zooming action of 100 Å is being inserted starting at frame 151 and taking 50 frames to complete the action.

2.3. EMOVIE IN ACTION

eMovie (Fig. 1) runs on Macintosh OS X (the X11 version, i.e. PyMOLX11Hybrid),¹ UNIX/LINUX and Windows. The user is presented with several buttons for interactive movie production and instructive help buttons assist first-time users (Fig. 1A). eMovie expects the user to be familiar with PyMOL and its graphical user interface (GUI), which is mostly self-explanatory. In PyMOL, each movie is treated as an ordered sequence of frames (pictures), to which particular actions are assigned. eMovie enables the user to enter actions in a modular way, generally by defining the starting point, the duration in frames, and the type of event that is required (Fig. 1C). Each action appears on an editable storyboard (Fig. 1B).

2.4. CREATING A MOVIE

To create a movie using eMovie, the user first loads the “actors”, or macromolecules, into PyMOL using the PyMOL GUI. Using the eMovie menu bar (Fig. 1A), the user chooses modular actions to add to different points in the movie. Modular actions include: scenes, rotations, zooms, fading, N->C rainbow colored backbone traces, and custom PyMOL commands. For example, a user inserts a zoom by clicking on ‘zoom’ and specifying a zoom of 100 Å starting at frame 151 and taking 50 frames to complete the action (Fig. 1C). Scenes store a distinct combination of view, colors, and representations and can be inserted to be recalled at any point in the movie. Morphs can also be created and inserted using the ‘Make morph’ and ‘Insert morph to movie’ buttons, but making a morph requires the subscription version of PyMOL called iPyMOL (version 0.99 recommended).

The breakthrough of eMovie is its storyboard feature (Fig. 1B). At any time the user can click on the “View Storyboard” button in the eMovie main menu to view the modular actions comprising the movie. The user can also click on any action and then click on ‘Edit action’ to edit it (for example change a zoom action from a zoom of 100 Å to one of 50 Å). Large groups of actions can be moved around in the movie using ‘Move a group of actions’, and actions can be removed entirely using ‘Delete selected action’. The storyboard provides powerful editorial control in an immediately responsive and user-friendly manner. When the movie is finished, the finished

¹ Switching from the Macintosh version of PyMOL (MacPyMOL) to the X11 version of PyMOL (PyMOLX11Hybrid) is simply accomplished by renaming the filename of MacPyMOL as PyMOLX11Hybrid (switching the name back reverts from PyMOLX11Hybrid to MacPyMOL). The authors find it useful to keep a copy of both versions on the Mac.

version is saved using the “Save eMovie” button, which the user has been using throughout the movie-making process to periodically save his or her movie.

2.4.1. *Exporting the movie to a traditional file format*

When the animation is finished, there are two options for playing it in a program other than PyMOL. One option is to use the ‘Export eMovie’ button (Fig. 1A) to export the movie as an image sequence and to subsequently merge the sequence to a common movie format (e.g. .mov, .gif or .mpeg) using programs such as Mencoder (UNIX and Windows), Graphic Converter (Macintosh OS X), Movie Maker (Windows), VideoMach (Windows), Adobe Premiere (Windows), or Berkeley encode_mpeg (UNIX or LINUX). A second option (for Macintosh users) is to save the finished eMovie using the PyMOL ‘File/Save Session’ feature; this saved session .pse file can then be opened in MacPyMOL and exported as File/Save_movie/QuickTime. Other programs can be used to apply titles, voice-over, music, labels and end credits.

2.5. CONCLUDING REMARKS

The availability of a storyboard-based, molecular movie-making tool such as eMovie has, without a doubt, the potential to affect the way science is communicated, as evidenced by the quick adoption of and positive response to the predecessor of eMovie, the movie.py PyMOL plug-in (<http://www.rubor.de/bioinf>). By making the creation of molecular movies more fluid through an editable storyboard, eMovie enables more scientists to take advantage of this media. An unfamiliar user can prepare an illustrative molecular movie for a presentation or a website within hours or even minutes.

eMovie can be downloaded from <http://www.weizmann.ac.il/ISPC/eMovie.html>, and PyMOL can be downloaded from <http://pymol.sourceforge.net>.

Sections 2.1, 2.2, 2.3, 2.4.1, 2.5, and 4.1 are reprinted from *Trends in Biochemical Sciences*, **32**, “eMovie: a storyboard-based tool for making molecular movies”, pp 199–204, Copyright (2007), with permission from Elsevier. For the full text including a more complete introduction to the field of molecular movie making and software that came before eMovie as well as a more detailed walkthrough of the eMovie workflow for creation of lengthy movies see the article in TiBS.

3. Proteopedia

3.1. INTRODUCTION

For all of the over 50,000 structures in the Protein Data Bank, rare is the non-structural biologist making use of the treasure of information. Because of the inherent complexity of a three-dimensional (3D) structure, structures can be hard to understand, especially for a non-structural biologist. As a result of this complexity, structural biology is still not in the mainstream of biology.

3D structures are most often communicated in two-dimensional (2D) media, namely scientific journals. In these journals 3D structures are compressed into 2D images, destroying the 3D information the crystallographer worked so hard to obtain. Molecular animations, such as those created with eMovie, are helpful in communicating 3D structures, but they are not the full solution because movies do not extend well to a large resource.

What's missing from structural biology is a way to communicate 3D structural information in a manner that is easy to understand. A resource with this quality would allow more effective communication between structural biologists and biologists, particularly by linking 3D structure to functional information in an intuitive manner.

Proteopedia is just this resource, and it has recently been made available on the web. In Proteopedia, descriptive text contains hyperlinks that, when clicked, change the orientation and representation of a 3D structure on the page in order to better explain a point made in the text. It is also a wiki-based web resource that allows the scientific community to easily contribute information via simple-to-use authoring tools. As a result, Proteopedia facilitates sharing and discussion among the scientific community and can help bring structural biologists and biologists to the same page.

Proteopedia is online at <http://www.proteopedia.org>, accessible via the popular operating systems and web browsers, and serving the scientific and educational community. There are already over 50,000 pages in the web resource, including pages on each of the entries in the PDB seeded with useful information and inviting an expert to contribute to them. Anyone from the scientific community can request an account to edit pages, but viewing pages does not require an account.

3.2. DESCRIPTIVE TEXT LINKED TO 3D VIEWS OF STRUCTURES

Perhaps the most powerful feature of Proteopedia is its capability to link descriptive text to 3D views of structures (a feature also implemented elegantly in the closed, proprietary viewer iSee⁸).

A user interested in Aricept[®], the widely used drug for treatment of the symptoms of Alzheimer's, could search for "Aricept" in Proteopedia, and find the Proteopedia page for the PDB entry 1eve (Fig. 2A). The PDB entry 1eve is the crystal structure of *Torpedo californica* acetylcholinesterase (TcAChE) complexed with Aricept[®]. Upon loading the Proteopedia page entitled 1eve, the user is greeted with a slowly revolving 3D structure of Aricept[®], also referred to as E2020, bound to the active site of TcAChE. The 3D structure is visualized using the molecular visualization applet Jmol.⁹ While structures are not presented in true 3D, the rotation of the structure on the screen creates the illusion of 3D.³

The user begins reading the text on the page. She or he reads that the X-ray structure of the E2020-TcAChE complex shows that E2020 has a unique orientation along the active-site gorge, and clicks on the green text 'unique orientation'. Immediately the 3D structure responds by transitioning to a scene that showcases the unique orientation of E2020, Aricept[®], along the active-site gorge (Fig. 2B). When the user reads that the orientation of E2020 extends from the anionic subsite (W84) of the active site, at the bottom, to the peripheral anionic site (near W279), at the top, he or she can click on the green links 'W84' and 'near W279' to see the respective residues labeled in the 3D scene (Fig. 2C,D). Reading that E2020 binds the active-site gorge tightly, but only through water intermediaries, the user clicks on the green link 'indirectly via solvent molecules' to view a scene illustrating the binding of E2020 in the active-site gorge (Fig. 2E).

We call these 3D views 'scenes' because they recall not just a particular view or orientation, but also a set of colors and representations and labels. At any time the user may zoom and rotate the 3D structure to explore it. The links can also be clicked in any order and still a smooth transition between 'scenes' results.

3.3. ADDING CONTENT AND EFFORTLESS CREATION OF 3D VIEWS

3.3.1. *How content is added*

Proteopedia is a 'wiki' web resource similar in spirit to Wikipedia.¹⁰ This means that pages in Proteopedia are not static but can be changed and improved by its users. All a user needs to do to edit a page is click on the 'edit this page' tab at the top of the page and begin editing the text of the page or inserting 3D scenes. Text editing is simple and performed in the same way as in Wikipedia because both websites are based on the open-source MediaWiki¹¹ software for wiki-sites. The 3D scenes are fashioned, also in a simple manner, using the Proteopedia Scene Authoring Tools. In depth and up-to-date editing help and explanations are available at <http://www.proteopedia.org/wiki/index.php/Help:Editing>.

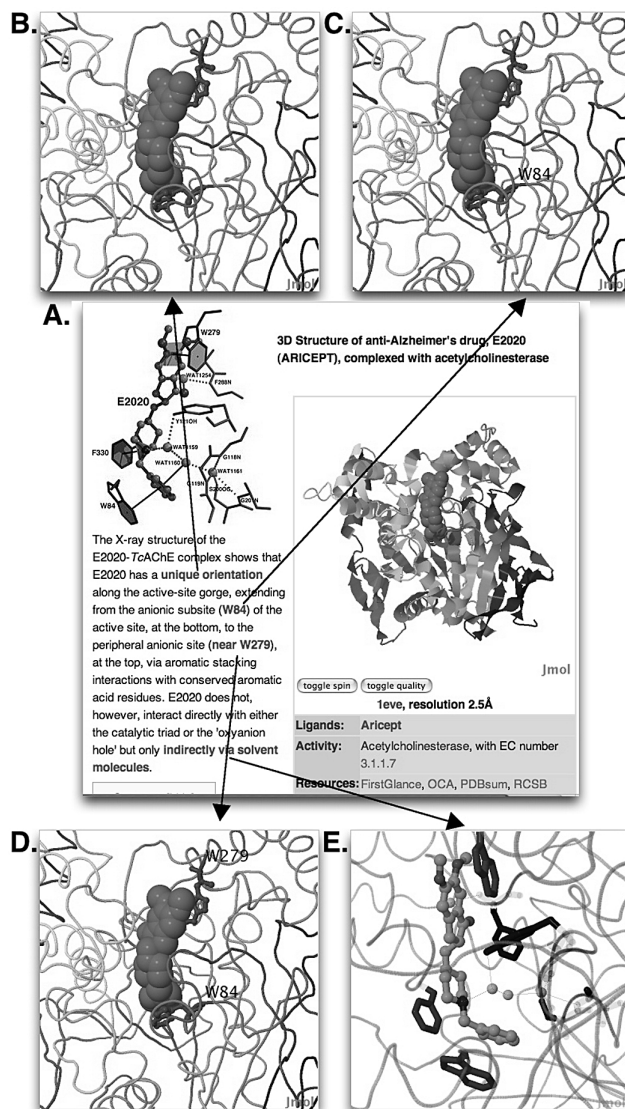


Figure 2. Proteopedia links descriptive text to 3D scenes. The arrows in this figure represent the changed Jmol visualization applet as a result of clicking on one of the green link (A) The page for the PDB entry 1eve containing the structure of AChE complexed with Aricept®. The molecule on the page is rotatable and zoomable and the green links change the appearance of the molecule when clicked. (A) The scene that loads when the user clicks on the green link 'unique orientation'. (B) W84 becomes labeled when the user clicks on the green link 'W84'. (C) W279 is labeled when the user clicks on the green link 'W279'. (D) Aricept® binds the active site of AChE tightly, but only through water intermediaries, this is show best when the user clicks on the green link 'indirectly via solvent molecules'.

3.3.2. 3D scenes in a snap

Perhaps surprisingly, 3D scenes are incredibly easy to create in Proteopedia. 3D scenes are created using the Proteopedia Scene Authoring Tools (SAT) (Fig. 3), which are accessible from every Proteopedia page by clicking on that page's 'edit this page' tab. The concept behind the SAT is such: A user loads a 3D structure into the SAT using the 'load molecule' tab (Fig. 3A). Following that, the user manipulates the 3D scene to the desired orientation, coloring scheme, representations, and labeling that will appropriately showcase

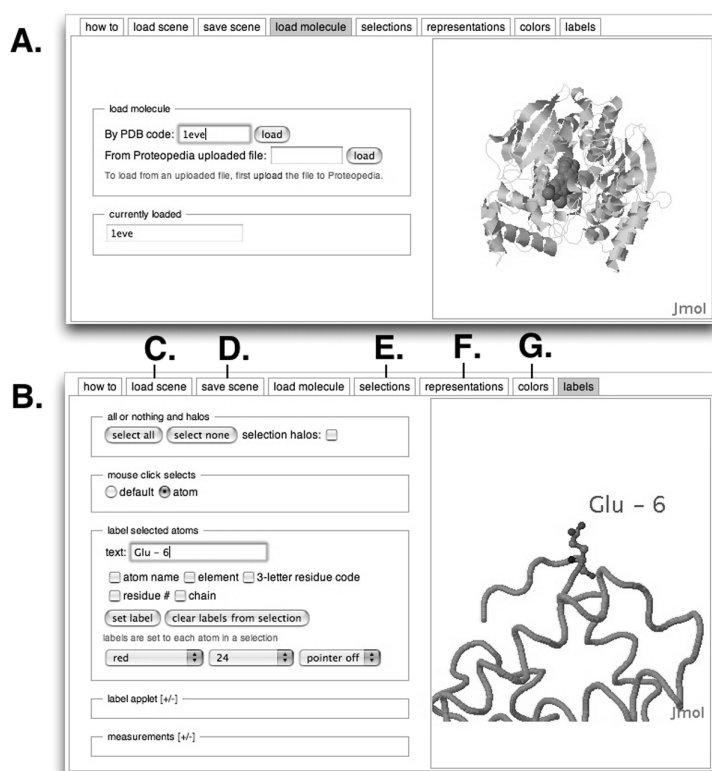


Figure 3. Two instances of the Proteopedia Scene Authoring Tools (SAT). (A) The SAT with the 'load molecule' tab active. The user has loaded the PDB file 1eve. (B) The SAT with the 'labels' tab active. The user has labeled a particular residue with the label 'Glu - 6' to highlight a mutation in hemoglobin that leads to the disease sickle-cell anemia. (C) The 'load scene' tab is used for loading existing scenes so they may be edited or used as a starting point for a new scene. (D) The 'save scene' tab allows the user to save a scene. (E) The 'selections' tab is used for choosing particular groups of atoms within the molecule. (F) The 'representations' tab is used for changing the representations of a particular group of atoms. (G) The 'colors' tab is used for changing the colors of a particular group of atoms, or the background color.

the intended point of the scene. When finished crafting the scene, the user saves the scene using the ‘save scene’ tab (Fig. 3D) and chooses a piece of text in the page to which to link the scene. That piece of text becomes a green link and recalls that scene when clicked.

In creating a scene, the user creates a still picture of sorts by saving a combination of colors, representations, labels, and viewpoint. When the scene is recalled by clicking the green link, the smooth transition that takes place is not a transition animation programmed by the user, but rather the transition animation is automatically handled by the software with each click of a green link.

The user sets the scene’s orientation using the mouse. Colors, representations, and labels often need to be set differently for a different groups of atoms within the 3D structure. Thus, first the user uses the ‘selections’ tab (Fig. 3E) to choose a select group of atoms, and then uses the ‘representations’ tab (Fig. 3F) to change the group’s representation, the ‘colors’ tab (Fig. 3G) to change the group’s coloring scheme, and the ‘labels’ tab (Fig. 3B) to add labels to select atoms within the group. Previously created scenes may be recalled and edited using the ‘load scenes’ tab (Fig. 3C).

A more detailed explanation of the SAT as well as the text-editing features of Proteopedia can be found at www.proteopedia.org/index.php/Help:Editing.

3.4. THE CHALLENGES OF A WIKI FOR THE SCIENTIFIC COMMUNITY

In order for a wiki-based resource to succeed in the scientific world, some changes must be made to the traditional wiki creed that suggests that anyone viewing the site should be able to edit any page, even anonymously.

3.4.1. *Members only: accounts restricted to the scientific community*

In Proteopedia, only registered users may edit pages. This contrasts with Wikipedia’s policy. To obtain a Proteopedia user account, a person must request one by clicking on ‘log in / request account’ at the upper right corner of the website. Account requests are approved only for members of the scientific community including scientists, educators, and students of science. In further contrast to Wikipedia, accounts are created in the users’ real names to allow for credit to be given to worthwhile contributions, as well as to encourage users to take responsibility for their edits. For now credit is given in the form of an automatic listing of “contributors” at the bottom of each Proteopedia page, but this model may evolve in the future to better ascribe credit to deserving authors.

3.4.2. *Handling inaccuracies, the dangers of a wiki*

It is hoped that by limiting user accounts to the scientific community, inaccurate contributions will be kept to a minimum. Additional protection features in Proteopedia common to other wiki-sites include the ability to protect specific contested pages from editing except from a select group of expert stewards. Users knowledgeable on a particular protein or subject can elect to receive emails whenever the page is altered, thereby forming a sort of editorial board for the page. The user community, in its use and browsing of the web resource, will also be expected to correct inaccuracies. The 'recent changes' page in Proteopedia displays a list of the most recent changes made to the database so that vigilant users can patrol the new changes to judge their merit. A history is kept of every edit to a page, and the page can be reverted to any particular past version with the click of a mouse.

3.4.3. *Catering to educators and supplementary material*

In another departure from the traditional wiki model, Proteopedia offers each registered user a section of Proteopedia to 'own'. Whenever a new user account is confirmed, a user page for that user is created in Proteopedia. That page, as well as all sub-pages of that page are protected from editing and can only be edited by the user for which that particular user page is named. While editing of these pages by anyone other than their 'owner' is disallowed, copying useful content from 'owned' pages to other Proteopedia pages is allowed and encouraged where doing so will improve the content of Proteopedia's main pages.

The protected pages allow educators to take advantage of Proteopedia's 3D visualization features by posting lectures for projection on Proteopedia and knowing that they will be protected from edits. Similarly, structural biologists seeking a powerful way to communicate newly published research can post supplementary material on Proteopedia and have it protected from editing.

3.5. MORE THAN 50,000 PAGES AND COUNTING

While still in its infancy, Proteopedia already contains over 50,000 pages. Included among these pages are pages for each of the entries in the PDB. These PDB entry pages have been seeded with content to make them already useful as well as to provide a platform for users to add content. Each PDB entry page contains a 3D visualization of the structure with green links highlighting features occasionally defined in the PDB file such as the active site and ligands. Among other useful information, each PDB entry page

contains the abstract from the structure's publication, inviting users to begin growing the page.

Proteopedia is not a copy of the PDB, however, in that the PDB entry pages are only part of the web resource. The next level up in the 'hierarchy' of pages would be the protein or molecule pages that have a more full description of the protein or molecule and also link to one or many relevant PDB entry pages. An example is the hemoglobin page, which gives a general overview of hemoglobin, as well as links to several PDB entry pages with various hemoglobin structures.

3.6. BEHIND THE SCENES: SOFTWARE

Proteopedia is based on an adapted version of the MediaWiki open source software for wiki-sites. Proteopedia integrates Jmol molecular visualization applets into the MediaWiki software via an adapted version of the Jmol MediaWiki Extension.¹²

3.7. DISCUSSION AND CONCLUSIONS

Proteopedia is growing daily with contributions. It is envisioned to be the first-stop resource for anyone interested in a particular protein or macromolecule with a solved 3D structure. Ideally each structural biology lab would have its own page on Proteopedia and the structural biology community as well as the scientific community at large would widely use the web resource. Only with increasing use over time can Proteopedia expect to satisfy its community of users and aid them in communicating structural biology to an ever-wider audience. The hope is that biologists will refer to Proteopedia to better understand the structure to function relationship of the proteins they are studying, and to better design experiments.

Proteopedia will continue to evolve and pursue future solutions for the intuitive presentation of 3D structural information. In its evolution, Proteopedia will continue to cater to its users by giving a high precedence to user-friendliness both in regards to users arriving to browse the resource and those arriving to contribute and add content.

ACKNOWLEDGEMENTS

EMOVIE

This study was supported by Autism Speaks, the Minerva Foundation, the Kalman and Ida Wolens Foundation, the Divadol Foundation, the Newman Foundation, a research grant from Mr. Erwin Pearl, the Bruce Rosen Foundation, the Kimmelman Center, the Israel Ministry of Science, Culture

and Sport grant for the Israel Structural Proteomics Center (ISPC), and the European Commission Sixth Framework Research and Technological Development Programme 'SPINE2-COMPLEXES' Project under contract No. 031220. E.H. is grateful to the K. Kupcinet 2006 Summer School (Weizmann Institute) for a fellowship. J.L.S. is the Pickman Professor of Structural Biology. We thank Anat Katz for very helpful discussion on the eMovie manuscript and Michael George Lerner, Seth Harris, Laurence Pearl, Tserk Wassenaar and Lieven Buts for their contributions to the original movie.py, and Warren DeLano – the creator of PyMOL – for useful suggestions.

PROTEOPEDIA

This study was supported by Autism Speaks, the Nalvyco Foundation, the Jean and Julia Goldwurm Memorial Foundation, the Benozziyo Center for Neuroscience, the Divadol Foundation, the Neuman Foundation, a research grant from Mr. Erwin Pearl, the European Commission Sixth Framework Research and Technological Development Programme 'SPINE2-COMPLEXES' Project under contract No. 031220 and 'Teach-SG' Project, under contract number ISSG-CT-2007-037198. JLS is the Morton and Gladys Pickman Professor of Structural Biology. E.H. is grateful to the Karyn Kupcinet Program and the Feinberg Graduate School (Weizmann Institute of Science) for a fellowship. The authors are very grateful to the Jmol and MediaWiki development teams for their support and development of their respective software packages. We also greatly appreciate the useful discussions with Gideon Schreiber, Yigal Burstein, Harry Greenblatt, John Moulton, Israel Silman, Eric Martz and Steven Brenner, as well as the generous use of content and images provided by Jane & David Richardson and David S. Goodsell.

References

1. Hodis, E., Schreiber, G., Rother, K. & Sussman, J. L., eMovie: A storyboard-based tool for making molecular movies, *TIBS* 32, 199–204 (2007).
2. Hodis, E., Prilusky, J., Martz, E., Silman, I., Moulton, J. & Sussman, J. L., Proteopedia - a scientific 'wiki' bridging the rift between three-dimensional structure and function of biomacromolecules, *Genome Biol.* 9, R121 (2008).
3. Levinthal, C., Molecular model-building by computer, *Sci. Am.* 214, 42–52 (1966).
4. Richardson, D. C. & Richardson, J. S., The kinemage: A tool for scientific communication, *Protein Sci.* 1, 3–9 (1992).
5. Sayle, R. A. & Milner-White, E. J., RASMOL: biomolecular graphics for all, *TIBS* 20, 374–376 (1995).
6. Stampf, D. R., Felder, C. E. & Sussman, J. L., PDBBrowse - a graphics interface to the Brookhaven protein data bank, *Nature* 374, 572–574 (1995).

7. Peitsch, M. C., Stampf, D. R., Wells, T. N. C. & Sussman, J. L., The Swiss 3D-Image collection and Brookhaven protein data bank browser on the World-Wide Web, *TIBS* 20, 82–84 (1995).
8. Abagyan, R., Lee, W. H., Raush, E., Budagyan, L., Totrov, M., Sundstrom, M. & Marsden, B. D., Disseminating structural genomics data to the public: From a data dump to an animated story, *TIBS* 31, 76–78 (2006).
9. Jmol.
10. Wikipedia.
11. MediaWiki.
12. Vervelle, N. Jmol MediaWiki Extension.