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Proteopedia: A status report on the collaborative, 3D web-encyclopedia of proteins and other biomolecules

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ABSTRACT

Proteopedia is a collaborative, 3D web-encyclopedia of protein, nucleic acid and other biomolecule structures. Created as a means for communicating biomolecule structures to a diverse scientific audience, *Proteopedia* (http://www.proteopedia.org) presents structural annotation in an intuitive, interactive format and allows members of the scientific community to easily contribute their own annotations. Here, we provide a status report on *Proteopedia* by describing advances in the web resource since its inception three and a half years ago, focusing on features of potential direct use to the scientific community. We discuss its progress as a collaborative 3D-encyclopedia of structures as well as its use as a complement to scientific publications and PowerPoint presentations. We also describe *Proteopedia*'s use for 3D visualization in structure-related pedagogy.

1. Introduction

With the solution of the first protein structure in 1958 by John Kendrew (Kendrew et al., 1958) came the inevitable problem of visualizing macromolecule structures. Kendrew's team approached this problem by constructing a physical model, and pictures of this model from various angles together served as a figure in the landmark publication. Computer-aided molecular visualization eventually superseded the building of physical models as the standard means to interpret and communicate a newly solved structure. However, a remarkable similarity with Kendrew's time remains: although computer-aided molecular visualizations can be easily shared electronically, when the time comes to publish, today's structural biologist still mimics the actions of Kendrew's team more than 40 years ago by capturing and submitting still images of a 3D model (now computer-generated) from various angles. Granted, many papers include stereoscopic images, but these are far from interactive, 3D representations. Model coordinates can also be downloaded and opened in the reader's molecular visualization application of choice, but the views and representations that have been carefully chosen for a figure are thus lost. Furthermore, most biologists without a background in structural biology are not familiar with molecular visualization applications. The notable exceptions to this apparent anachronism in communicating the authors' viewpoints of 3D macromolecule structures, namely "3D interactive journal figures", began in 1992 with David and Jane Richardson's Kinemage molecular illustrations (Richardson and Richardson, 1992). Currently there are several alternative approaches, including the proprietary iSee platform (Abagyan et al., 2006; Lee et al., 2009); a method for embedding interactive 3D figures within PDF files (Kumar et al., 2008, 2010); and Jmol display (Hanson, 2010; Jmol, 2010), which in various forms includes the IUCr Jmol enhanced toolkit (McMahon and Hanson, 2008), *Protein Science*'s implementation (Palmer and Matthews, 2009), Molecules in Motion (Reichsman, 2010) and *Proteopedia*'s Interactive 3D Complements [U1] (n.b. the symbols [U1], [U2] etc. refer to the *Proteopedia* URLs listed in Table 1).

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The difficulties encountered in visualizing and communicating macromolecular structures motivated the creation of *Proteopedia* [U2] as a collaborative, 3D web-resource for presentation of biomolecule structures (Hodis et al., 2008). *Proteopedia* aims to allow the community of structural biologists, as well as the scientific community as a whole, to intuitively and easily communicate 3D structural annotations to a broad scientific audience. Use of the *Proteopedia* web resource is free, requires no downloads or installations (other than Java, standard on most computers) and makes contribution of structural annotations relatively easy. Interactive, 3D models of biomolecule structures are displayed, using Jmol, adjacent to descriptive text containing links. When clicked, these links evoke changes in the orientation, representation, and labeling of the 3D model, thus illustrating the points made in the text. In this status report we describe advances in *Proteopedia* since its creation almost four years ago. For the original communication describing the *Proteopedia* web resource the reader is referred to (Hodis et al., 2008). Here we detail recent progress in *Proteopedia*'s use:

- as a 3D web-encyclopedia of protein and other biomolecule structures
- for interactive visualizations to complement scientific publications and Microsoft PowerPoint presentations
- as a pedagogic tool for teaching biomolecule structure and function in the classroom

Structure communication on the web through a collaborative, 3D encyclopedia of biomolecule structures.

Table 1
Referenced *Proteopedia* URLs.

Number in text	URL	Proteopedia page/article
[U1]	proteopedia.org/w/Interactive_3D_Complements_in_Proteopedia	*Proteopedia*'s Interactive 3D Complements
[U2]	proteopedia.org	*Proteopedia*'s Main Page
[U3]	proteopedia.org/w/4hhb	4hhb
[U4]	proteopedia.org/w/Hemoglobin	Hemoglobin
[U5]	proteopedia.org/w/Proteopedia:Structure_Index	*Proteopedia*'s Structure Index
[U6]	proteopedia.org/w/Peroxisome_Proliferator-Activated_Receptors	Peroxisome proliferator-activated receptors (PPAR)
[U7]	proteopedia.org/w/Angiotensin-converting_enzyme	Angiotensin-converting enzyme (ACE)
[U8]	proteopedia.org/w/Plant_Viral_Protein_p19_Suppression_of_RNA_Silencing	Plant Viral Protein p19 Suppression of RNA Silencing
[U9]	proteopedia.org/w/Phosphoinositide_3-Kinases	Phosphoinositide 3-Kinases (PI3K)
[U10]	proteopedia.org/w/Cation-pi_interaction	Cation-π interactions
[U11]	proteopedia.org/w/Quality_assessment_for_molecular_models	Quality assessment for molecular models
[U12]	proteopedia.org/w/Hydrogen_in_macromolecular_models	Hydrogen in macromolecular models
[U13]	proteopedia.org/w/Lac_repressor	Lac repressor
[U14	proteopedia.org/w/Citrate_Synthase	Citrate synthase
[U15]	proteopedia.org/w/Recoverin	Recoverin, a calcium-activated myristoyl switch
[U16]	proteopedia.org/w/Mechanosensitive_channels:_opening_and_closing	Mechanosensitive channels: opening and closing
[U17]	proteopedia.org/w/Forms_of_DNA	Forms of DNA
[U18]	proteopedia.org/w/Helices_in_Proteins	Helices in proteins
[U19]	proteopedia.org/w/Large_Ribosomal_Subunit_of_Haloarcula	Large ribosomal subunit of *Haloarcula*
[U20]	proteopedia.org/w/Ramachandran_Plot	Ramachandran plot
[U21]	proteopedia.org/w/HMG-CoA_Reductase	HMG-CoA reductase
[U22]	proteopedia.org/w/Proteopedia:Video_Guide	*Proteopedia*'s Video Guide
[U23]	proteopedia.org/w/Help:Contents	*proteopedia*'s help pages
[U24]	proteopedia.org/w/Proteopedia:How_to_Make_a_Page	*Proteopedia*'s How to make a page
[U25]	proteopedia.org/w/Proteopedia:Table_of_Contents	*Proteopedia*'s Table of Contents
[U26]	proteopedia.org/w/HIV_Protease	HIV-1 protease
[U27]	proteopedia.org/w/Acetylcholinesterase	Acetylcholinesterase
[U28]	proteopedia.org/w/AChE_inhibitors_and_substrates	AChE inhibitors and substrates
[U29]	proteopedia.org/w/Atorvastatin	Atorvastatin (Lipitor)
[U30]	proteopedia.org/w/Metabolic_Disorders	Metabolic disorders
[U31]	proteopedia.org/w/Pharmaceutical_Drugs	Pharmaceutical Drugs
[U32]	proteopedia.org/w/Pharmaceutical_Drug_Targets_and_Diseases	Pharmaceutical Drug Targets and Diseases
[U33]	proteopedia.org/w/Avidin	Avidin
[U34]	proteopedia.org/w/Workbenches	*Proteopedia*'s Workbench feature
[U35]	proteopedia.org/w/User:Janice_C._Telfer/Group_B_SRCR_domains	Group B SRCR domains (I3DC)
[U36]	proteopedia.org/w/User:Oleg_Kovalevskiy/Engineered_mutants_of_HlyIIR	Engineered mutants of HlyIIR (I3DC)
[U37]	proteopedia.org/w/3btp	*Agrobacterium* virulence complex VirE1–VirE2 (I3DC)
[U38]	proteopedia.org/w/Journal:JBIC:6	Sco proteins are involved in electron transfer processes (I3DC)
[U39]	proteopedia.org/w/Journal:JBIC:8	A hydrogen-bonding network formed by the B10-E7-E11 residues of a truncated hemoglobin from *Tetrahymena pyriformis* is critical for stability of bound oxygen and nitric oxide detoxification (I3DC)
[U40]	proteopedia.org/w/JBIC	List of *JBIC* I3DCs in *Proteopedia*
[U41]	proteopedia.org/w/Serine_Proteases:_A_Tutorial_of_Chymotrypsin,_Trypsin_and_Elastase	Serine proteases: a tutorial of chymotrypsin, trypsin and elastase
[U42]	proteopedia.org/w/Structural_templates	Structural templates
[U43]	proteopedia.org/w/Teaching_Scenes,_Tutorials,_and_Educators'_Pages	Central repository for 3D structure tutorials
[U44]	proteopedia.org/w/Teaching_Strategies_Using_Proteopedia#Student_Authoring_of_Temporary_Proteopedia_Pages:_Sandboxes	Student Authoring of Temporary Proteopedia Pages: Sandboxes
[U45]	proteopedia.org/w/GFP	Green fluorescent protein
[U46]	proteopedia.org/w/Triose_Phosphate_Isomerase	Triose phosphate isomerase
[U47]	proteopedia.org/w/Group:SMART:Teams	Students Modeling A Research Topic (SMART) Teams
[U48]	proteopedia.org/w/Group:SMART:A_Physical_Model_of_the_β2-Adrenergic_Receptor	A SMART Team's page: A Physical Model of the β2-Adrenergic Receptor