

# A molecule undergoing simulation

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The focus of the study, conducted through the means of VIM, was directed towards Ubiquity, a regulatory protein found in nearly every eukaryotic tissue and associated with the function of degradation of defective and superfluous proteins in the organism. A special emphasis was given to the graphical analysis of protein backbone conformation and secondary structure, general atom distribution, and hydrophobic versus hydrophilic behavior and its connection with polar and non-polar region distribution. As a culmination of the study, it was concluded that the structure of the Ubiquity molecule adheres to the scientific principles of protein structure and function.

**INTRODUCTION** The current study focused on the graphical analysis of the structure of the Ubiquity protein molecule using the VIM computer program. VIM is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VIM is designed for modeling, visualization, and analysis of biological systems such as proteins, nucleic acids, and lipid belayed assemblies.

It may be used to view more general molecules, as VIM can read standard Protein Data Bank (PDB) files and display the contained structure. VIM provides a wide variety of methods for rendering and coloring a molecule: simple points and lines, CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, cartoon drawings, and others. VIM can be used to animate and analyze the trajectory of a molecular dynamics (MD) simulation. In particular, VIM can act as a graphical front end for an external MD program by displaying and animating a molecule undergoing simulation on a remote computer. Ubiquity is a small regulatory protein that has been found

in almost all cells with nuclei eukaryote). It directs proteins to recycling and other functions.

Ubiquitination is a post-translational modification (an addition to a protein after it has been made) where Ubiquity is attached to a substrate protein. The addition of Ubiquity can affect proteins in many ways: It can signal for their degradation via the protease, alter their cellular location, affect their activity, and promote or prevent protein Ubiquitination is carried out in three main steps: activation, conjugation, and ligation, performed by Ubiquity-activating enzymes (E1s), Ubiquity-conjugating enzymes (E2s), and ubiquity aliases (E3s), respectively. The result of this sequential cascade binds Ubiquity to lysine residues on the protein substrate via an isopeptide bond or to the amino group of the protein's N-terminus via a peptide bond.

The purpose of this investigation was to analyze Ubiquity protein structure, with special emphasis given to backbone conformation and secondary structure, general atom distribution, and hydrophobic versus hydrophilic behavior and its connection with polar and non-polar region distribution, with the final goal of getting acquainted with the VIM program and to confirm whether or not the structure of the Ubiquity molecule adheres to the scientific principles of protein structure and function. The study was conducted through the means of the VIM program, particularly through the creation of various graphical representations using the "Graphics" menu, due to the superb visualization, in-depth structure display, and visual analysis options and techniques provided by this program. MATERIALS AND METHODS adding the Molecule A PDB file (1UBQ. PDB) that contains the

atom coordinates of the Ubiquity molecule was retrieved from the ARCS Protein Data Bank.

A VIM session was started. In the VIM Main window, File New Molecule... Fig. 1 (a)) was chosen.

Another window, the Molecule File Browser window (Fig. 1 (b)), appeared on the screen. The Browse...

(Fig. 1 (c)) button was used to find the file “ 1 UBS. PDP” file. The Load (Fig. 1 button was then pressed. General Graphical Analysis of the Molecule VIM was used to display the molecule in various ways using the Graphical Representations tab. Each representation was defined by four main parameters: the selection of atoms included in the representation, the drawing style, the coloring method, and the material. The selection determined which part of the molecule was drawn, the drawing method defined which graphical representation IS used, the coloring method gave the color of each part of the representation, and the material determined the effects of lighting, shading, and transparency on the representation.

To display the Ubiquity molecule in order to utilize the Graphical Representations techniques, in the VIM Main window the Graphics Representations... Menu item was chosen. The Graphical Representations window appeared with the current default representation displaying the molecule. The graphical analysis of the Ubiquity protein was further enhanced by the options of the Selections (Fig. 2(a)) tab. Using the Selections tab options, parts of the molecule of particular interest were highlighted by specifying them in the Selected Atoms text entry.

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In order to do that, in the Graphical Representations window choose the Selections tab (Fig. 2(a)) was chosen. In section Singleton's (Fig. (b)), the list of possible selections that were typed in the Selected Atoms text entry was found.

The Apply button was hit in order to display the typed selection in the window where the Ubiquity Lucile was pictured using AD graphics. The section Keen. Ford (Fig. 2(c)) of the Selections tab, contained the properties that were used to select parts of a protein with their possible values.

In this investigation, this selection was particularly used to display the locations of various protein residues on the Ubiquity molecule. Utilizing these options, various graphical representations of the Ubiquity protein molecule were created and analyzed and the techniques of the VIM visualization program were acquainted with. Graphical Analysis Of particular Structural Areas Of the Molecule After a mineral graphical study of the Ubiquity molecule was conducted and the VIM program was familiarized with, special emphasis was given to particular structural areas of the protein with the goal to ultimately validate whether or not the structure of the Ubiquity molecule adheres to the scientific principles of protein structure and function. Those structural areas included general atom distribution, backbone conformation and secondary structure, hydrophobic versus hydrophilic behavior and its connection with polar and non-polar region distribution, as well as various types of protein residues and heir locations with the Ubiquity molecule. The Microsoft Powering program was later used to display the created graphical representations with their respective titles and color keys for the elements that were highlighted utilizing the Selections tab. General Atom Distribution

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In order to create a graphical representation of the general atom distribution of the Ubiquity protein molecule, in the Draw Style tab of the Graphical Representations menu the Coloring Method was changed to “ Element” and the Drawing Method was changed to “ CAP”. Then, in the Selections tab, in the Selected Atoms text entry atom names of carbon, oxygen, nitrogen, and sulfur were typed, hitting the Apply button after each atom entry and the Create Rep button before each new atom entry.

In addition, it was made so the protein backbone was visible in the representation. This was done by changing the Coloring Method to “ Color ICY’ (color white) and the Drawing Method to “ New Ribbons” in the Draw Style tab. Then, in the Selections tab, the Create Rep button was hit, and the word “ backbone” was typed in the Selected Atoms text entry, then the Apply button was pressed. Backbone Conformation and Secondary Structure Secondary structure defines the shape of the backbone of the protein. In order to create a secondary structure graphical representation of the Ubiquity molecule, the protein backbone was first made visible in the representation.

This was done with a similar procedure as before, by changing the Coloring Method to “ Color ID’ (color white) and the Drawing Selected Atoms text entry, then the Apply button was pressed. After that, the Drawing Method was changed to “ New Cartoon”. In the Selected Atoms text entry, secondary structure types of an alpha helix, beta sheet, and a 3-10 helix ere typed, hitting the Apply button after each secondary structure type entry and the Create Rep button before each new entry. In addition, the color was changed before each entry, with the color yellow identifying an alpha helix, green

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highlighting a beta sheet, and purple signifying a 3-10 helix. Three representations Were created to display Ubiquity backbone conformation.

With a similar procedure, the protein backbone was first made visible In white and the backbone conformation was displayed using the same procedure as for the secondary structure, but instead of alpha helix, beta sheet, and 3-10 Elis, the words typed into the Selected Atoms text entry were coil conformation and turn conformation. The other two graphical representations depicted residue conformation angles, one displaying “ phi” angles and the other one displaying “ SSI” angles. The procedure was again commenced with the displaying of the backbone in white. After that, the Drawing Method was changed to “ Tube” and the “ phi” and “ SSI” words typed in the Selected Atoms text entry were pulled from the Keywords section below. The Coloring Method remained “ Color ID” for the entire time, with active angles, positive angles, and angles that equal zero signified by different colors. In order to make sure only negative “ SSI” angles were highlighted, for example, “  $SSI < 0$ ” was type into the Selected Atoms text entry. Hydrophobic Versus Hydrophilic Behavior and Polar and Non-polar Region Distribution For this part of the investigation, four graphical representations in total were created. Two were created to display hydrophilic versus hydrophobic behavior in the Ubiquitin molecule, and two were created to display the polar and non-polar region distribution of the protein.

The ackbone was made visible in white repeating the same procedure as above for all the representations, while the Coloring Method was kept as “ Color ID”. For the first two pairs Of representations, hydrophobic and Nan-  
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polar regions were identified with blue while hydrophilic and polar regions were identified with the color red. Following similar procedures as the studies above, words “ hydrophobic”, “ hydrophilic”, “ polar”, and “ non-polar” were entered in the Selected Atoms text entry. The Drawing Method was set to “ CAP” for one representation out of the two in each pair, while the second representation had a Drawing Method of “ Dotted” for the hydrophobic versus hydrophilic case, with the second representation in the polar versus non-polar case having a “ Surf” Drawing Method.

**RESULTS** In this display of the general atom distribution of the Ubiquity protein molecule (Figure 3) created using the VIM computer visualization program, carbon appears to be the dominant element. The numbers of oxygen and nitrogen atoms seem to be in an about equal ratio, each being about half the number of carbon atoms in the protein. There appears to be only one sulfur atom for the entire Ubiquity molecule. The carbon atoms are clustered towards the center of the protein while the oxygen atoms appear to lie more to the outside of the molecule, with nitrogen atoms being dispersed evenly throughout the whole protein. Also, the carbon atoms can be seen attached to the backbone via bonds, therefore forming the academics of the molecule.

All the other atoms, however, appear to be not bonded on the most part, especially the oxygen atoms, most of which are floating freely outside the molecule. **Backbone Conformation** In this display of the backbone residue conformation created using the VIM computer visualization program (Figure 4), about half of the backbone sides appears to be in either turn or coil conformation. There is about an equal amount of backbone residue in turn <https://assignbuster.com/a-molecule-undergoing-simulation/>



conformation as there is in coil conformation in the Ubiquity molecule. It also appears that the majority of backbone residue in coil conformation and the majority of residue in coil conformation are clustered on opposite ends of the protein. This is a display of the backbone residue conformational angles, created using the VIM computer visualization program (Figure 5).

Here the distributions of different residue conformation angles of both types, phi and SSI, were marred. The conformation angles were differentiated by negative, positive and those equal to zero. Judging from the graphical representation, it appears that the backbone's SSI residue conformation angles are mostly negative while the phi residue conformation angles are mostly positive. In addition, the graphical representation showing phi conformation angles also has a region where the angle is equal to zero, while the other representation does not have such an angle. Secondary Structure This is a display of the secondary structure of the backbone of the Ubiquity rotten molecule, created using the VIM computer visualization program (Figure 6). Depicted here are the respective locations of the areas where the protein backbone is folded in the form of an alpha helix, beta sheet, or a 3-10 helix. Judging from the graphical representation, the area where the protein backbone is in the form of an alpha helix is opposite from the area where it is folded as beta sheets.

It also appears that the beta sheet secondary structure dominates the protein backbone, while all the regions of beta sheet backbone folding seem to be clustered together. The backbone form of a 3-10 helix mess to occur the rarest in the Ubiquity molecule out of the three types of secondary structure form. Hydrophobic versus Hydrophilic Behavior This is a display of <https://assignbuster.com/a-molecule-undergoing-simulation/>

the location of hydrophobic and hydrophilic regions within the Ubiquity protein molecule, created using the VIM computer visualization program (Figure 7). All the hydrophobic academics of the molecule appear to be clustered towards the center of the protein while all of the hydrophilic academics of the Ubiquity molecule appear to be pushed towards the outside of the protein. There is no intermixing between the hydrophobic and hydrophilic regions of the molecule. Polar and Non-Polar Region Distribution This is a display of the location of polar and Nan-polar regions within the Ubiquity protein molecule, created using the VIM computer visualization program (Figure 8). The distribution of polar and non-polar regions within the protein bears a striking resemblance to the distribution of hydrophobic and hydrophilic regions within the molecule.

The same as in the graphical representations above, all the non-polar academics of the molecule appear to be clustered towards the center of the protein while all of the polar outside of the protein. There is again no intermixing between the hydrophobic and hydrophilic regions of the molecule. DISCUSSION Overall, the goals of this investigation were fully met and the main purpose of the study of demonstrating the adherence of ubiquity tin's structure to general scientific principles of protein function was accomplished. The VIM was described and concluded to be a molecular visualization program used for displaying, animating, and analyzing large bimolecular systems using 3-D graphics and built-in scripting, and designed for modeling, visualization, and analysis of biological systems such as proteins, nucleic acids, and lipid belayed assemblies. The VIM program was fully acquainted with.

From loading the data for the Ubiquity protein to mastering the use of tools, techniques and options available in the Graphics menu of the program, optimal graphical representations of the Ubiquity molecule were created. The graphical analysis of Ubiquity protein backbone conformation and secondary structure, general atom distribution, and hydrophobic versus hydrophilic behavior and its connection with polar and non-polar region distribution was inducted using the VIM program, with the graphical representations created yielding desired results to prove the purpose of this study. All of the graphical representations of the selected structural areas constructed during the experiment adhere to the principles of protein science.

Specifically, starting with the general atom distribution displayed in Figure 3, carbon seems to be the dominating element. This is scientifically supported since proteins are known to consist at least two thirds out of the carbon element. The presence of oxygen, nitrogen and sulfur is also justified by the fact that all here are essential components of Organic molecules. Oxygen atoms are pushed to the outside of the protein and appear to be not bonded due to the fact that they are part of the water molecules that typically surround cell proteins like Ubiquity. The protein backbone conformation graphics examined the location of turn and coil conformation as well as various phi and SSI angles. A turn is an element of secondary structure in proteins where the polypeptide chain reverses its overall direction while a coil conformation is a structural motif in which 2-7 alpha-helices are coiled together like the trends of a rope.

Both don't occur consistently the protein and don't occur simultaneously in one region of the backbone, explain the fact the in the graphical representation each compromised only about one fourth of the protein backbone in addition to being located on opposite ends of the ubiquity molecule. As far as the phi and SSI representations go, they're also scientifically accurate. Phi angles measure the central bond between nitrogen and carbon while SSI angles measure the central bond between two carbon atoms. The reason the negative and positive angle distributions of phi and SSI angles appeared significantly opposite is because the two measure the angles between two completely different pairs of atoms. The graphical representation of backbone secondary structure of the Ubiquity molecule is also scientifically accurate, with alpha helixes and especially beta sheets being the dominant backbone forms, with 3-10 also being intact. The ubiquity graphical representations demonstrating hydrophobic versus hydrophilic behavior and its connection with polar and non-polar region distribution also helped prove the adherence of Ubiquity structure to the principles of protein science. First Of all, the distribution Of hydrophobic regions Of the protein bared a striking resemblance to the distribution of non-polar regions in the molecule, while the same goes for hydrophilic and polar regions.

Also, while the hydrophobic and non-polar regions were clustered towards the center of the protein, the hydrophilic and polar areas were pushed towards the outside of the Ubiquity molecule. This is not surprising, considering hydrophobic and non-polar characteristics are practically the same thing, both repelled by the polar water molecules and yearning

towards the center away from the waters that typically surround protein molecules. At the same time, hydrophilic and polar characteristics, also similar, are attracted to the water molecules on the outside. Protein molecules are even specifically known to contain a hydrophobic core, making the following structural representations of the Ubiquitin molecule ideal for illustrating the scientific laws of protein structure. Through the thorough examination of these structural areas of the protein and their correspondence with general scientific knowledge, it can be scientific principles of protein structure and function. If the study can be updated, other areas of protein structure would be put through in-depth graphical analysis in order to once again prove Ubiquitous structural adherence to scientific law.