

Wenxiang: a web-server for drawing wenxiang diagrams

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Received 15 September 2011, revised 16 October 2011; accepted 23 October 2011.

ABSTRACT

The wenxiang diagram was proposed to represent α -helices in a 2D (two dimensional) space (Chou, K.C., Zhang, C.T., Maggiora, G.M. *Proteins: Struct., Funct., Genet.*, 1997, 28, 99-108). It has the capacity to provide more information in a 2D plane about each of the constituent amino acid residues in an α -helix, and is particularly useful for studying and analyzing amphiphilic helices. To meet the increasing requests for getting the program of generating wenxiang diagrams, a user-friendly web-server called “Wenxiang” has been established. It is accessible to the public at the web-site <http://www.jci-bioinfo.cn/wenxiang2> or <http://icpr.jci.edu.cn/bioinfo/wenxiang2>. Furthermore, for the convenience of users, here we provide a step-to-step guide for how to use the Wenxiang web-server to generate the desired wenxiang diagrams.

Keywords: Amphiphilic Helix; Helix-Helix Interaction; Hydrophobic; Hydrophilic; 2D Diagram; Wenxiang Diagram; Helical Wheel Diagram

1. INTRODUCTION

The α -helix is one of the most basic and fundamental elements in protein structure [1]. Owing to their regularity, α -helices have had an immense influence on our understanding of protein structure. Also, owing to their elasticity, many marvelous biological functions of proteins can be revealed through the low-frequency accordion-like motions of α -helices (see, e.g., [2-4] and a comprehensive review [5]).

Using graphical or diagrammatic approaches to study biological systems can provide an intuitive picture or useful insights for helping analyzing their complicated mechanisms, as demonstrated by many studies on a series of important biological topics, such as enzyme-catalyzed reactions [6-9], protein folding kinetics [10,11],

inhibition of HIV-1 reverse transcriptase [12-14], inhibition kinetics of processive nucleic acid polymerases and nucleases [15], drug metabolism systems [16], protein attribute prediction [17,18], protein sequence evolution [19], among many others.

Since the “pen-and-paper space” and most of the “publication space” are two-dimensional (2D) space, it is desirable to represent the 3D structures of α -helices on a 2D plane. In this regard, two different kinds of diagrams are usually used to represent α -helices. One is called the “helical wheel diagram” [20], and the other called “wenxiang diagram” [21]. The name of the latter came from the fact that it looks like a coil-like incense used in China to repel mosquitoes, *i.e.*, Chinese “蚊香” (pronounced as “wenxiang”). For its shape and appearance, click the link <http://wapedia.mobi/zh/%E8%9A%8A%E9%A6%99>.

According to its original definition [21], a 2D wenxiang diagram is generated by a conical projection of an α -helix onto a plane perpendicular to its axis (**Figure 1**). For a rigorous definition of an α -helix’s axis, see [22]. In the 2D wenxiang diagram each amino acid residue is represented by a circle with a letter to indicate its single character code, while its location in the 2D plane is defined by both an angle around the helix’s axis and the distance from the center, the intersection point between the 2D plane and the helix’s axis, as elaborated in [21].

As a 2D representation, the wenxiang diagram has the following features: (i) able to show the relative locations of the amino acids in an alpha-helix regardless how long it is; (ii) able to indicate the direction of an alpha-helix; and (iii) having the capacity to provide more information about each of the constituent amino acid residues in an α -helix [21].

With these features, the wenxiang diagram can provide an intuitive and easily visualizable picture in a 2D space that characterizes the disposition of different residue types in an α -helix.

As is known, except for transmembrane helices, α -helices in globular proteins are generally amphiphilic, *i.e.*, consist of two types of residues, hydrophobic and hydrophilic, with the number of each type being roughly

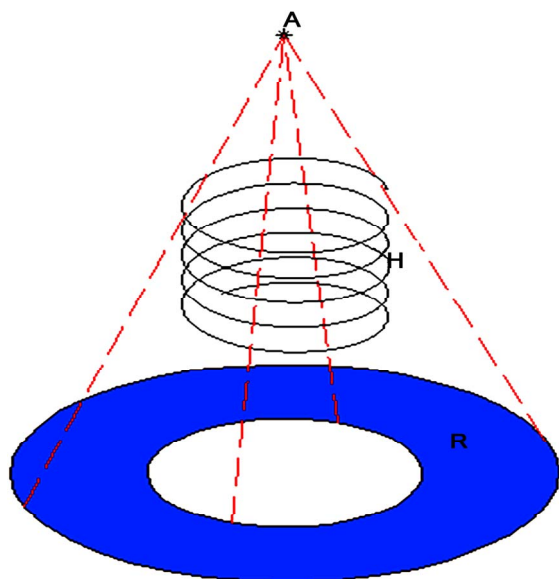


Figure 1. Conical projection of a helix H onto a plane perpendicular to the helix H. The dashed lines represent the radiating lines from the apex A. The image of helix H on the projection plane is within the ring area R: the closer the part of helix H is from the apex A, the further away its image is from the center of the ring R.

equal. Wenxiang diagrams are particularly useful to help gain insights into the interactions among amphiphilic helices or between proteins that contain amphiphilic helices [23,24].

Recently we have received many requests for the program of generating wenxiang diagrams. To address these requests in a unified manner, we have established a web-server by which one can easily generate the wenxiang diagram for any α -helix according to its amino acid sequence, as described below.

2. EQUIPMENT

You need a computer with access to the Internet and a web browser.

3. PROCEDURE

You should follow the guide below to generate the wenxiang diagram for an α -helix.

1) Go to the web page at <http://www.jci-bioinfo.cn/wenxiang2> or <http://icpr.jci.edu.cn/bioinfo/wenxiang2>, and you will see the top page of the **Wenxiang** web-server on your computer screen, as shown in **Figure 2**.

2) Click the [Read Me](#) button to see the user's instructions, which can be elaborated via the following steps.

3) Either type or copy and paste the α -helix amino acid sequence (in single letter code) into the input box at the lower centre of **Figure 2**. If you are not sure about the input format, click on the button [Example](#) right

above the input box to see the format of an acceptable input sequence.

4) Click on the [Black & White](#) button to generate a black-and-white wenxiang diagram (**Figure 3**), where **hydrophobic** residues are shown by "black-filled circles with white characters" while **hydrophilic** residues by "open circles with black characters". It will take about 20 seconds before the desired diagram is completely shown on the screen.

5) Or alternatively, click the button [Color](#) to generate a color wenxiang diagram (**Figure 4**), where **hydrophobic** residues are shown by "red-filled circles with white characters" while **hydrophilic** residues by "blue-filled circles with black characters".

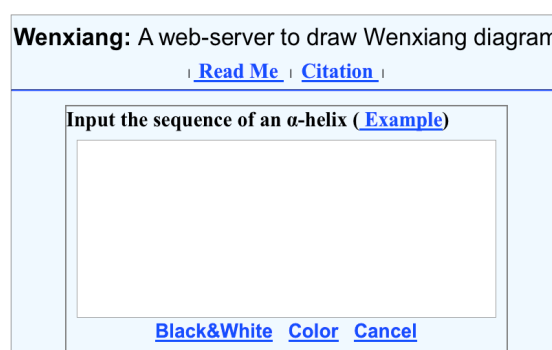


Figure 2. A screenshot of the top page of the **Wenxiang** web-server at <http://www.jci-bioinfo.cn/wenxiang2> or <http://icpr.jci.edu.cn/bioinfo/wenxiang2>.

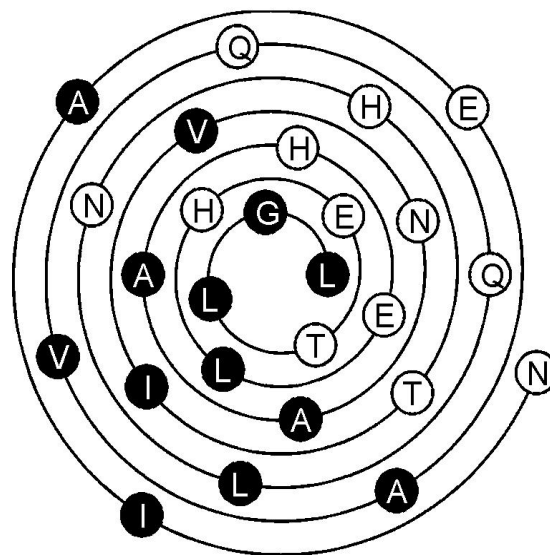


Figure 3. The black-and-white wenxiang diagram generated by clicking the [Black & White](#) button of the web-server for the input sequence taken from the [Example](#); the "black-filled circles with white characters" represent the **hydrophobic** residues, while the "open circles with black characters" **hydrophilic** residues.

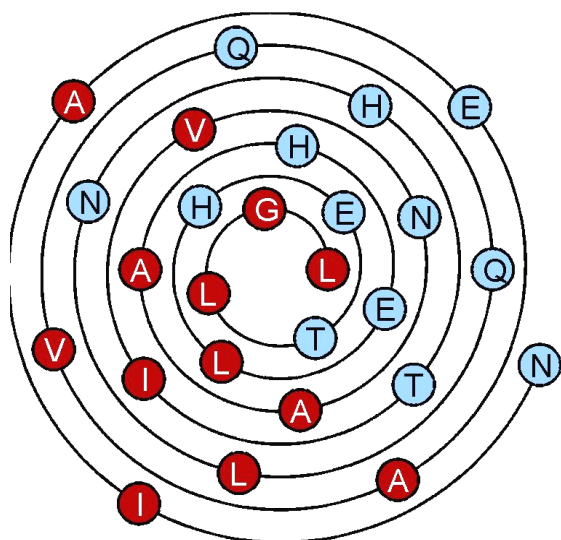


Figure 4. The color wenxiang diagram generated by clicking the [Color](#) button of the web-server for the same input sequence as in [Figure 3](#). The “red-filled circles with white characters” represent **hydrophobic** residues, while the “blue-filled circles with black characters” represent the **hydrophilic** residues.

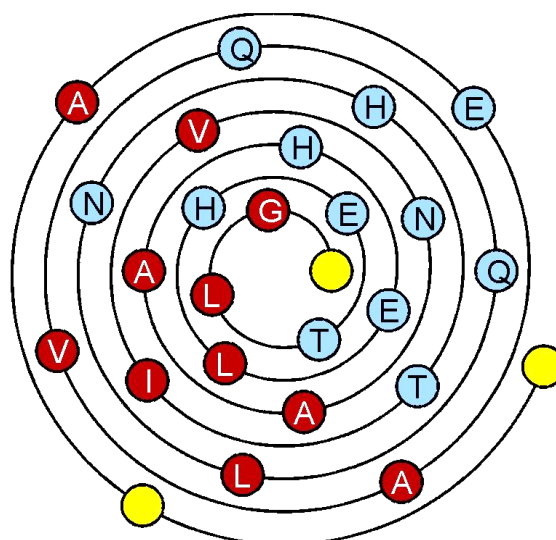


Figure 6. The color wenxiang diagram generated by clicking the [Color](#) button of the web-server for the same input sequence in [Figure 5](#). The three “yellow-filled circles” represent the three invalid codes at the 1st, 2nd, and last positions of the sequence, respectively.

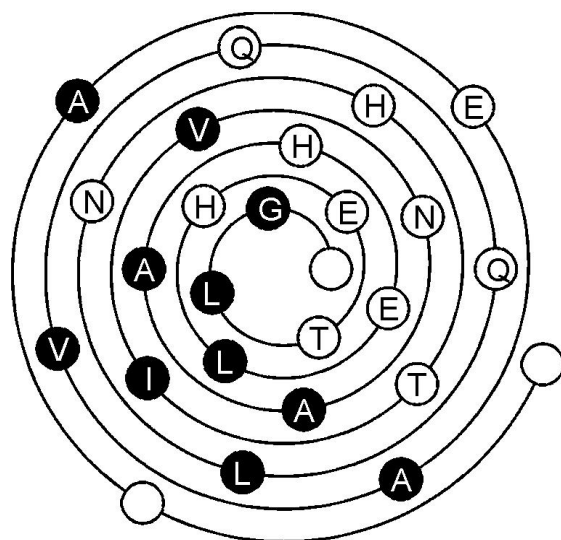


Figure 5. The black-and-white wenxiang diagram generated by clicking the [Black & White](#) button of the web-server for the input sequence XXAEAVQQ-LNHTIVNAAHELHETLGX that contains invalid codes in its 1st, 2nd and last positions. The three “open circles” represent the three invalid codes at the 1st, 2nd, and last positions, respectively.

6) To save the wenxiang diagram, click it with the right mouse button.

7) Click on the [Citation](#) button to find the relevant papers that document the detailed development of wenxiang diagram and some of its applications.

4. DISCUSSION

The valid codes for a native α -helix should be within the 20 characters ACDEFGHIKLMNPQRSTVWY, which represent 20 native amino acids, respectively.

If your sequence contains some invalid codes, after clicking the [Black & White](#) button, a warning message will occur on the screen. If you still want to generate the wenxiang diagram, just click the [OK](#) button. However, the wenxiang diagram thus generated will contain some “open circles” with each corresponding to one of the invalid codes. For example, for the input sequence XXAEAVQQ-LNHTIVNAAHELHETLGX where the first two codes and the last one are invalid, the wenxiang diagram thus generated will look like the one shown in [Figure 5](#).

The similar situation will also occur when clicking the [Color](#) button to generate the color wenxiang diagram for the above invalid sequence, in which case each of the invalid codes will be shown by a “yellow-filled circle” as shown in [Figure 6](#).

The wenxiang diagrams thus generated for non-native helices that contain invalid codes may give you some flexibility for studying hypothetical α -helices.

5. ACKNOWLEDGEMENTS

This work was supported by the grants from the National Natural Science Foundation of China (No. 60961003), the Key Project of Chinese Ministry of Education (No. 210116), and the Department of Education of Jiangxi Province (No. GJJ11557).

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