

# INTERACTION OF 3D MODELS FROM PROTEIN DATA BANK BASE WITH UCSF CHIMERA AND WORK IN BLENDER SOFTWARE

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**Abstract:** Protein Data Bank features affordable standardized high-quality 3D models of biological molecules. In certain cases it is necessary standardized 3D geometry models to be used for specific tasks, which are set requirements for the direct integration. This is required in cases of creation of simulations, animation of processes, interactive visualization or presentations. The implementation of such processes is complex and require precision and correct selection of the technological tools that promote the realization of the work.

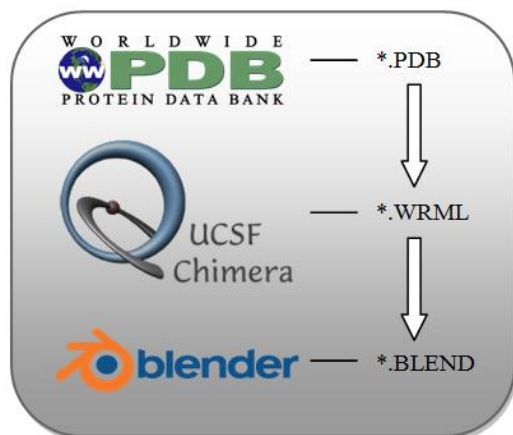
**Keywords:** PDB, 3D, CHIMERA, BLENDER

## 1. Problem discussion

Protein Data Bank has all the necessary resources of digitized 3D models of biological molecules [1 - 6]. The information provided in the database is very detailed and well structured. It meets all modern requirements and international standards [7 - 9]. When the need to perform tasks requiring the use of standardized 3D geometry models \*.PDB specialized technology software applications are applied such as Chimera and Blender. The need for 3D visualization combined with a detailed description of molecules, positions, surface, volume, etc. requires specialized platform UCSF Chimera. [10 - 13]. In a further realization of simulation processes and presenting animation, the functional capabilities of Blender software is applied [14 - 17].

## 2. Objective and research methodologies

The interaction between the Protein Data Bank, UCSF Chimera and Blender software requires certain conditions guaranteeing the successful work with 3D PDB models. Fig. 1 shows the defined technological features necessary in the transfer of information data in three stages.

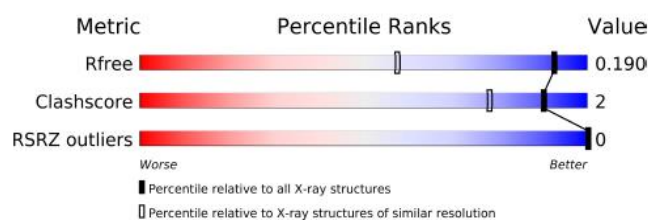


**Fig.1. The interaction between Protein Data Bank, UCSF Chimera, and Blender software**

The aim of this study is to establish the optimal capabilities using the resources of the Worldwide Protein Data Bank, specialized application UCSF, and 3D design potential of Blender software.

The study uses a 3D model of the Ultra high resolution dickerson-drew dodecamer b-dna with PDB ID: 4C64 and resolution 1.32 Å (reported) [18].

WWPDB validation of 4C64 is shown on Fig.2.



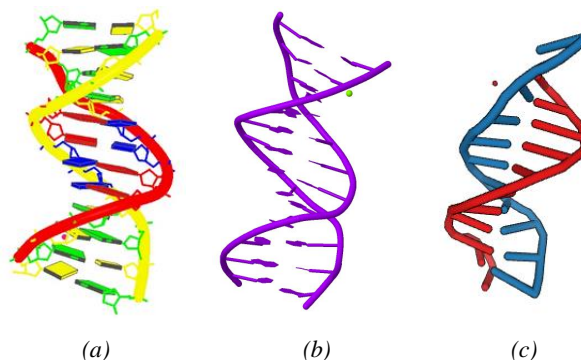
**Fig. 2. WWPDB validation of 4C6C**

The table 1 summarizes the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3, 2, 1$  and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	12	
1	B	12	

**Table1. Quality of chain of 4C64**

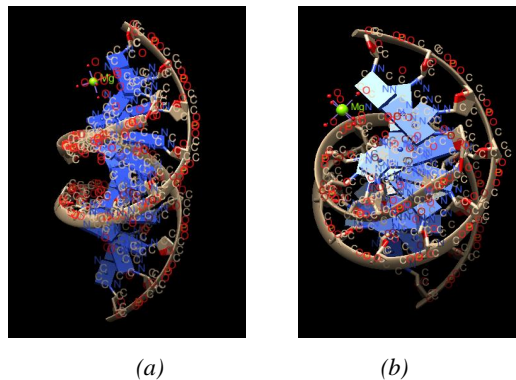
Fig. 3 shows the three visualization options on the Internet platform of Worldwide Protein Data Bank, respectively: static graphic, JSmol and PV (in Browser).



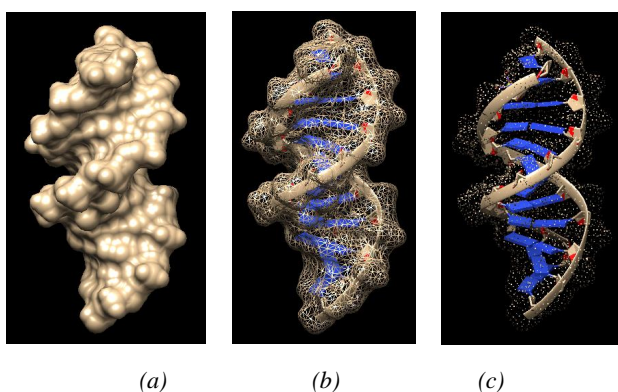
**Fig.3. Worldwide Protein Data Bank visualization of 3D Model with PDB ID: 4C64 (a) Static graphic, (b) JSmol and (c) PV (in Browser).**

Internet platform Wpdb provides limited visual ability to work with 3D models, resulting in the need to import the geometry of the models in an environment of UCSF Chimera. This will enable a

detailed consideration of the positioning of the participating elements (Fig. 4), and the total surface volume (Fig. 5).



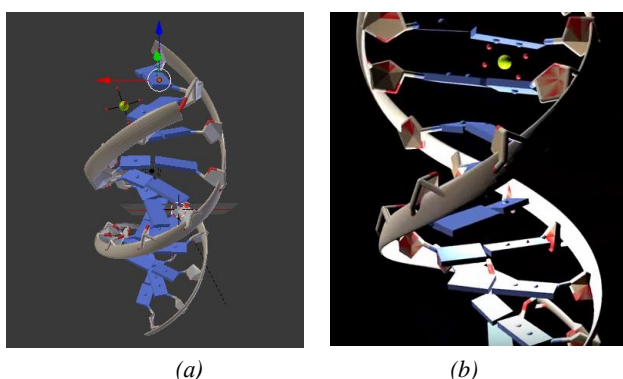
**Fig.4. UCSF Chimera visualization of 4C64 + label of elements (a) full view (b) zoomed view**



**Fig.5. UCSF Chimera visualization of surface of 4C64 (a) Solid, (b) Mesh and (c) Dot.**

In carrying out animation 4C6C, the 3D model is exported from Chimera (VRML file type) and is imported in Blender software in \*.wrl file.

FIG. 6 shows the pattern of 4C6C environments Blender software, where the necessary actions to obtain the final animation are done.



**Fig.6. Animating of 4C6C (a) Blender view (b) Blender rendered view**

The resulting animation Ultra high resolution dickerson-drew dodecamer b-dna with PDB ID: 4C64 was publicly presented and can be seen online at:

<https://www.youtube.com/watch?v=ze-38ZnvYa0>.

### 3. Conclusion

The use of the advantageous features of UCSF Chimera and Blender software build fully functioning system of opportunities for work with standardized 3D models of molecules provided free by Worldwide Protein Data Bank.

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