

PRINCIPLE OF INTERACTION BETWEEN WORLDWIDE PROTEIN DATA BANK AND BLENDER SOFTWARE

Phd Tihomir Dovramadjiev

Mechanical Engineering Faculty, Industrial Design Department - Technical University of Varna, Bulgaria.

tihomir.dovramadjiev@gmail.com

Abstract: For the needs of the medical, biomedical and other professionals the Protein Data Bank (PDB) is the principal place - a repository of 3D structured data of biological molecules. For visualization, simulation and animation of various processes it is necessary the 3D models of proteins and nucleic acids to be combined with proper 3D graphics platform. Such is Blender, which has some big advantages in 3D graphics, with suitable functional capabilities and is fully accessible to consumers.

Keywords: PDB, 3D, BLENDER

1. Problem discussion

Protein Data Bank [1 - 6] is a resource designed for the needs of modern biology, providing data about the biological molecules. The storage is fully accessible and impresses with the vast amount of information necessary to the practical needs and at level of the official science. The database is constantly updated and supplemented and a number of organizations have a huge contribution to this (NIH, NSF, EBI, PDBe, PDBj, RSCB, BMRB, etc. [7 - 9]), as well as scientist from all over the world. Except in 3D computer format the information about the provided biological molecules is announced in scientific journals and also is applied to the required specifications [10 - 12]. Data on the molecules is usually obtained by X-ray crystallography or MRI spectroscopy. World Protein Data Bank Organization require scientists to submit data on the structure of the PDB. When in an appropriate form, the information provides researchers with the opportunity to have biological molecules to be used specifically to the particular needs. In certain cases these are the realization of computer simulations and animations for whose implementations appropriate 3D graphics programs like Blender are used [13 - 16].

2. Objective and research methodologies

This study aims to optimize the workflow between the Worldwide Protein Data Bank and Blender software.

For compatibility between the Protein Data Bank and Blender software is necessary to activate Atomic Blender - PDB in 3D program. This enables the import of PDB (Protein Data Base) files and the export of objects to PDB. The activation of Atomic Blender - PDB is by going through the menu file, selection of user preferences, select the add-ons and Import - Export, where is the application (Fig.1).

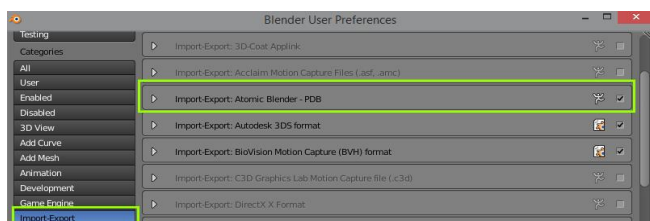


Fig. 1. Activation of Atomic Blender – PDB in Blender

For the specific requirements of the study the models will be imported and animated in <<The von Willebrand Factor A3 domain binding region of type III collagen (PDB ID : 4GYX)>> and <<The NAC domain of ANAC019 in complex with DNA, gold derivative (PDB ID : 3SWM)>> [17, 18]. 3D models of PDB files are provided by their selection in certain specific way of work in Protein Data Bank internet resource (Fig. 2).

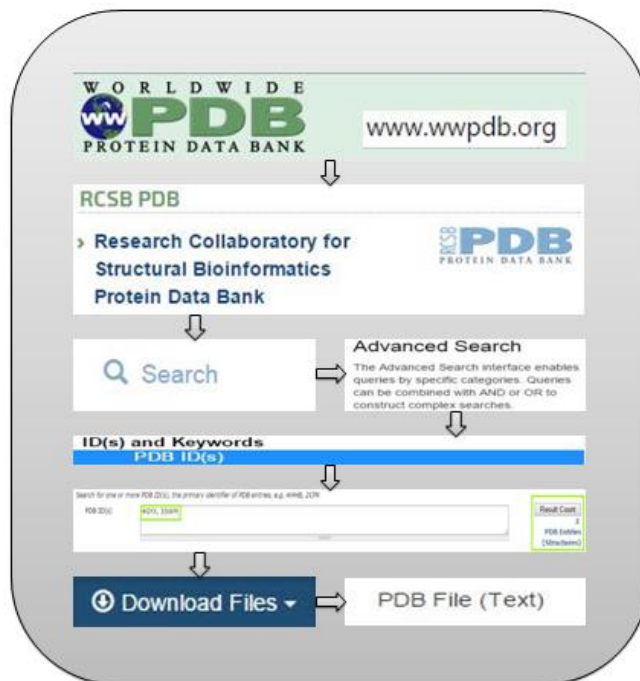


Fig.2. Providing of PDB 4GYX and 3SWM models

WWPDB validation of 4GYX and 3SWM are shown on Fig.3 and Fig. 4.

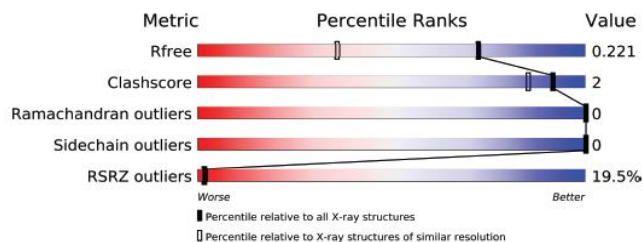


Fig. 3. WWPDB validation 4GYX

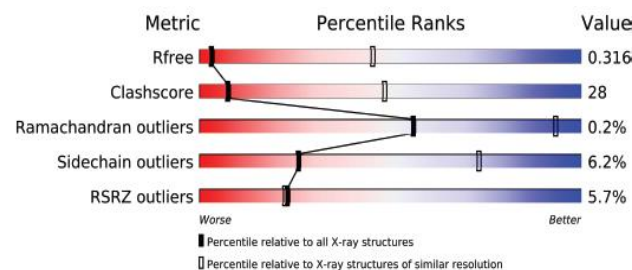


Fig. 4. WWPDB validation 3SWM

The tables below summarize the geometric issues observed across the polymeric chains and their fit to the electron density (Table 1: 4GYX; Table 2: 3SWM). The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	31	
1	B	31	
1	C	31	

Table 1. Quality of chain of 4GYX

Mol	Chain	Length	Quality of chain
1	A	174	
1	B	174	
1	C	174	
1	D	174	
2	E	26	
3	F	26	

Table 2. Quality of chain of 3SWM

When importing the Protein Data Bank files (*.pdb) default definitions of models are selected (Fig.5.)

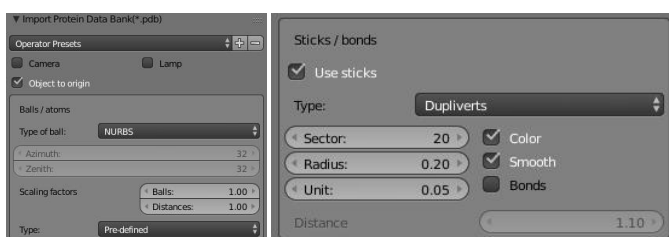


Fig. 5. Definitions of imported files (*.pdb)

Fig.6. 4GYX and Fig.7. 3SWM shows the directly imported 3D PDB models in Blender software.

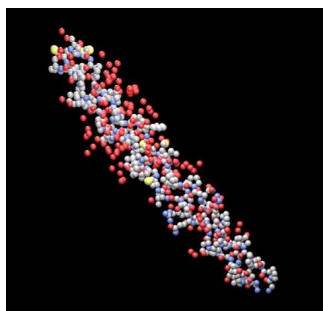


**Fig.6. General view
4GYX 3D model**

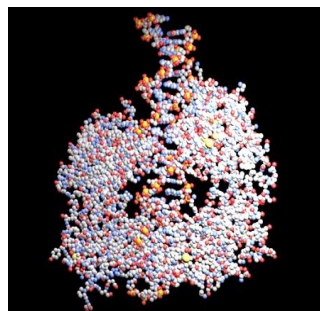


**Fig.7. General view
3SWM 3D model**

For the animation of the obtained 3D models the necessary adjustments of lighting, camera, and movement are made. The results were presented publicly and can be viewed online on the Internet at:

<https://www.youtube.com/watch?v=O1cb6FYS2gE> 3a <<The von Willebrand Factor A3 domain binding region of type III collagen (PDB ID : 4GYX)>> and <https://www.youtube.com/watch?v=3Jy3wwWsmrk> 3a <<The NAC domain of ANAC019 in complex with DNA, gold derivative (PDB ID : 3SWM)>>.

3. Conclusion

The relationship between the Protein Data Bank and Blender software is important in making additional graphical, simulated and animated processes for the needs of certain studies and

presentations. Knowing the principle of interaction, consistency and specific features is necessary condition for successful realization of the work. Opportunities provided by Blender software are in positive progress in implementing the compatibility of the program to the needs of Worldwide Protein Data Bank.

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