MS03-1-8 Interactions Between Hydrophilic Polymers and Biomacromolecules
#MS03-1-8

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Abstract
Hydrophilic polymers of polyethyleneglycol type are often used as precipitants for crystallization of bio-macromolecules. It is the reason why many of experimental structures deposited in Protein databank [1] show PEG type polymers bound on the protein surface. We inserted these structures in the Database of Protein-Polymer Interactions (DPPI) [2].
The DPPI contains presently 3667 PDB structures of bio-macromolecules (proteins and nucleic acids) complexed with PEG type fragments at least 4 monomers long (-OCC-OCC-OCC-OCC-O-). The script of the program PYMOL [3] allows quick identification and inspection of configurations of polymer chain bound on the protein surface. It automatically zooms and displays distances of all relevant interatomic contacts between polymer and protein. As some proteins bind more polymer chains, the DPPI contains many thousands experimentally verified interactions. To help quick inspection of many situations, the DPPI users deposit the pictures in special directory using the command PNG
Correct localization of the polymer chains on the protein surface does not lie in the centre of crystallographer's interest. This is the reason why, we can meet some evident misinterpretations. Of course, it is not allowed to make any corrections in the PDB file. Instead, the user can write the corresponding comment into the text box inserted in the picture similarly as it is shown in the Figure.
Visual inspection of the DPPI provides surprisingly high number of various types of protein-polymer interactions. Classification of these interactions is a useful background for explaining the success of the poly(ethyleneglycol)-type polymers in many economically important applications in the industry, science, medicine and pharmaceutics, e.g. crystallization of proteins, protection of drugs against enzymatic cleavage, development of antifouling surfaces, etc.
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References
1. wwPDB consortium Protein Data Bank: Nucleic Acids Research, (2018) 47, D520-D528. DOI: 10.1093/nar/gky9492. Hašek, J., Z. Kristallogr. (2011) 28, 475-480. DOI: 10.1524/9783486991321-0773. Schrödinger, L., & DeLano, W. (2020). Program PyMOL. Retrieved from http://www.pymol.org/pymol
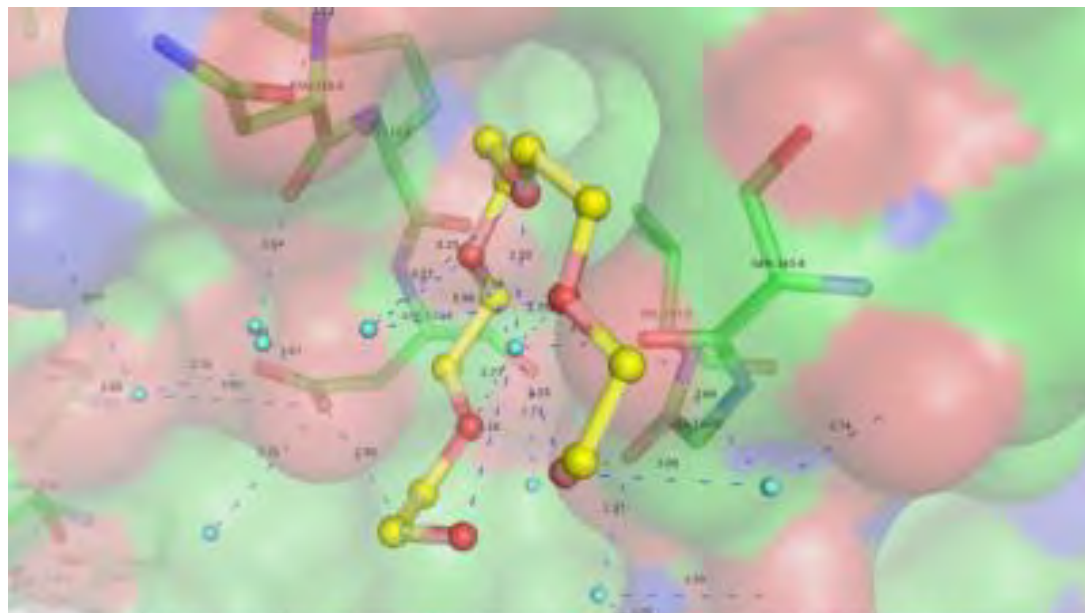
File name of the picture **1Y33-15P-O6 C=O-M@O6 inhibited-Subtilisin.png**
Meaning: **1Y33**=PDB code, **15P**=name of ligand, **O6**=six oxygens of PEG bind the protein, **C=O-M@O6** = protein carbonyl binds metal atom trapped in the center of six ether oxygens of PEG. As the modelled oxygen lies in the plane of the six oxygens, it is probably natrum **ion Na⁺**.