

Algorithms in Structural Bioinformatics

I.Z. Emir and E.D. Chrysina

Assignment 2

Announced: 24.05.2023 / Deadline: Friday 02.06.2023 23:59

The 3D structure of the human serotonin receptor was determined in the absence and in the presence of serotonin (PDB id: 7e2x, 7e2y).

Please see the following link: <https://www.ebi.ac.uk/pdbe/news/serotonin-ruffling-feathers>, read the relevant paper by Xu, P., Huang, S., Zhang, H. *et al.* Structural insights into the lipid and ligand regulation of serotonin receptors. *Nature* **592**, 469–473 (2021). <https://doi.org/10.1038/s41586-021-03376-8> and go through very carefully the information/figures provided in PDBe regarding this entry (PDB id: 7e2y)

1. Report on the following regarding 7e2y:
 - a. Method by which the 3D structure was determined and the Resolution
 - b. Number of chains and number of residues in each chain
 - c. Which are the ligands that are present in the structure
2. Use the molecular visualization software Chimera-X <https://www.cgl.ucsf.edu/chimerax/> to prepare different figures of the overall structure of the complex:
 - a. A figure presenting the secondary structure elements of the protein coloured by chain
 - b. A figure presenting the chemical distinct molecules in the structure
3. Determine the R.M.S.D. between the human receptor structure deposited with PDBe determined experimentally and the chicken one predicted with AlphaFold.
 - a. Over all atoms
 - b. Over Ca atoms
 - c. Using the secondary structure elements only