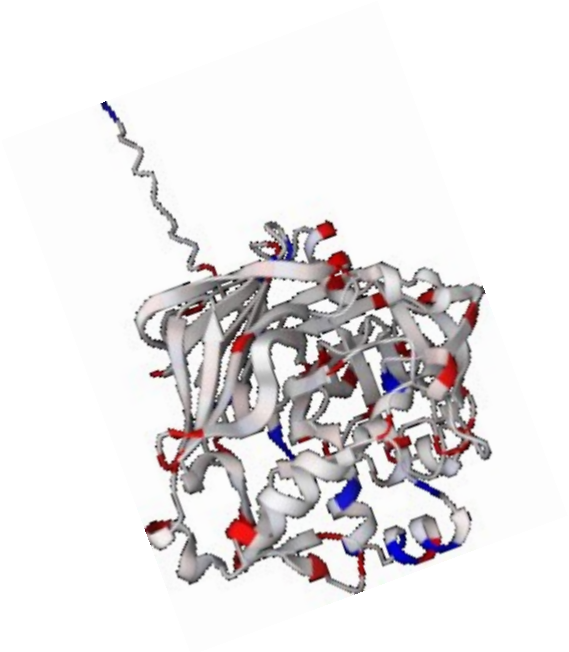
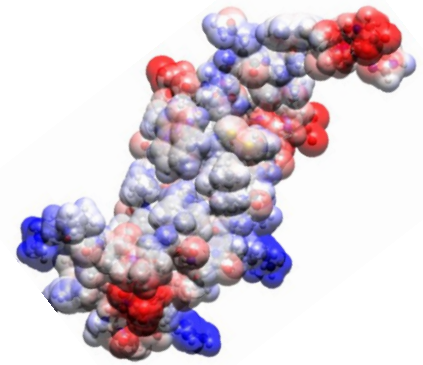
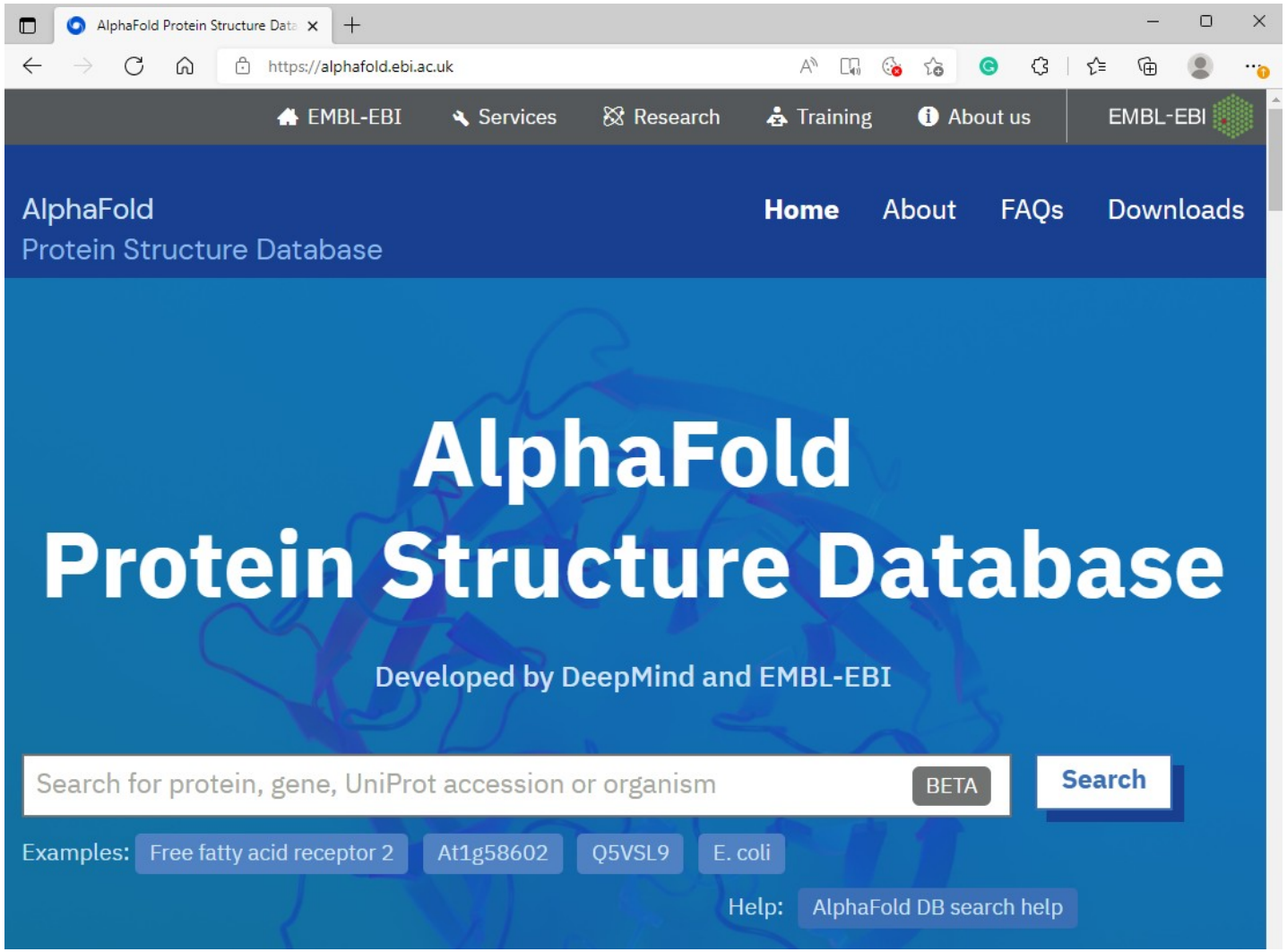
Charges
Partial atomic charges for AlphaFold structures





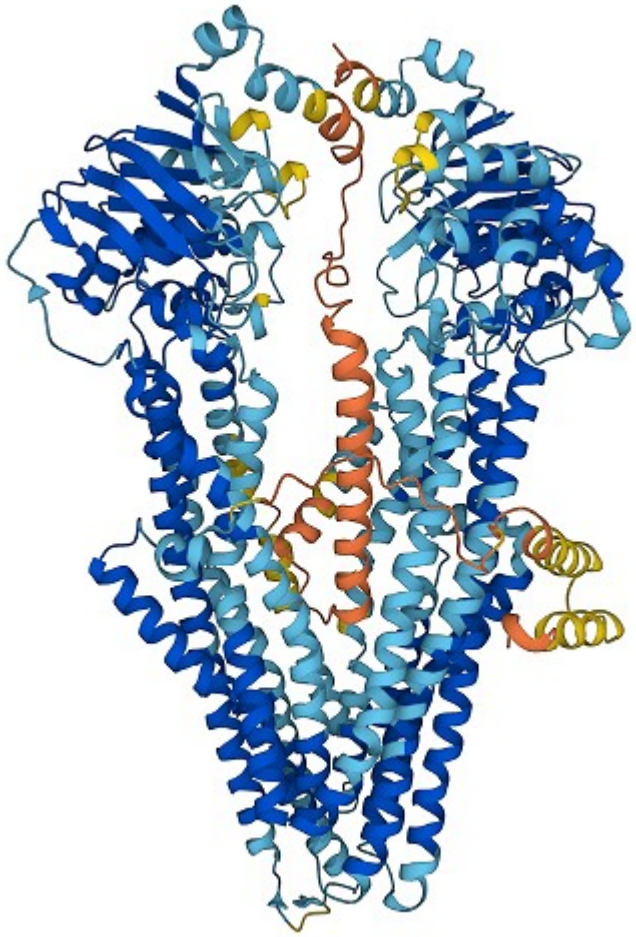
Central European Institute of Technology
BRNO | CZECH REPUBLIC

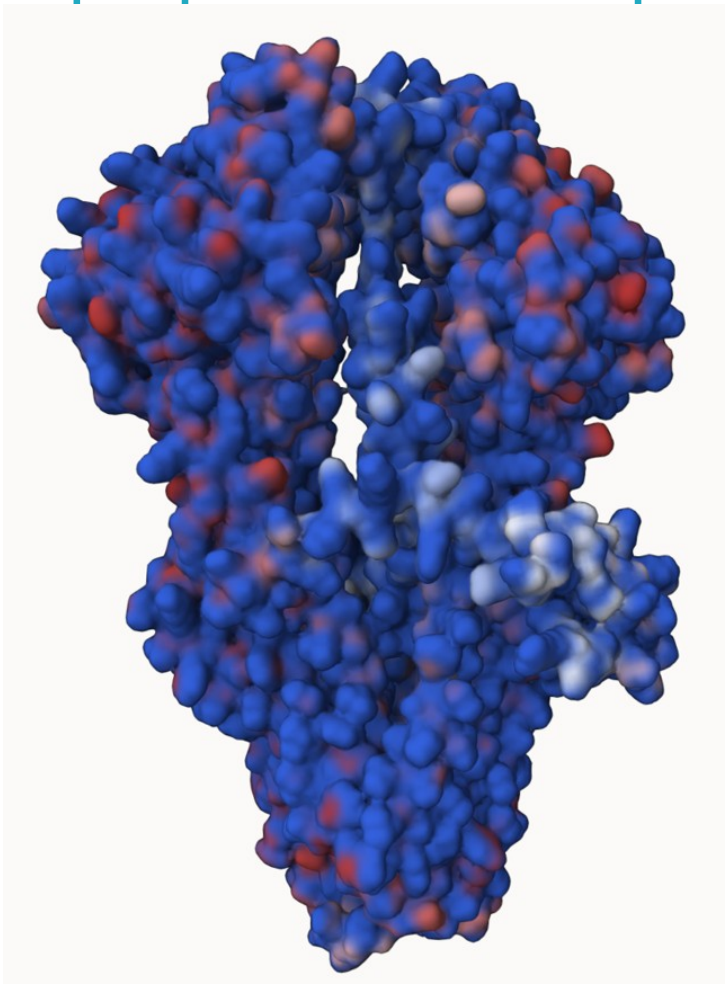
AlphaFoldDB – predicted protein structures



~ 200 M protein structures

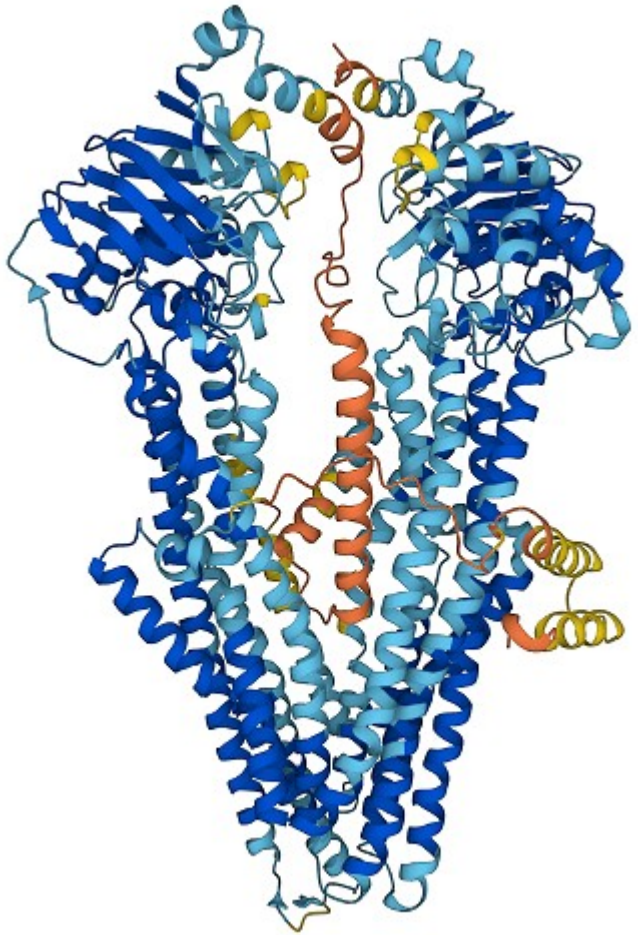
Why partial atomic charges?
They show the chemical properties of the predicted structures

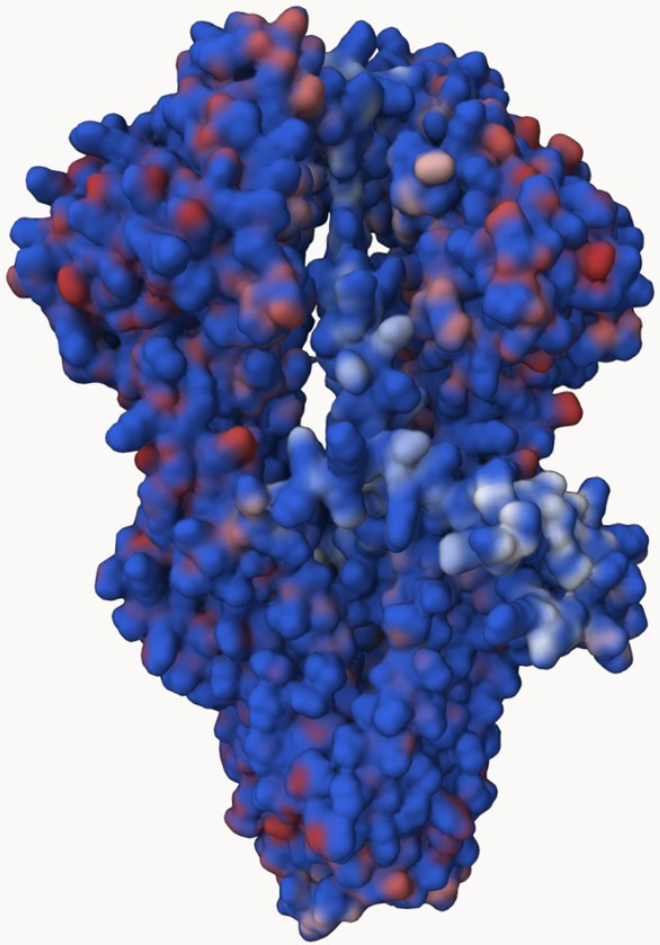


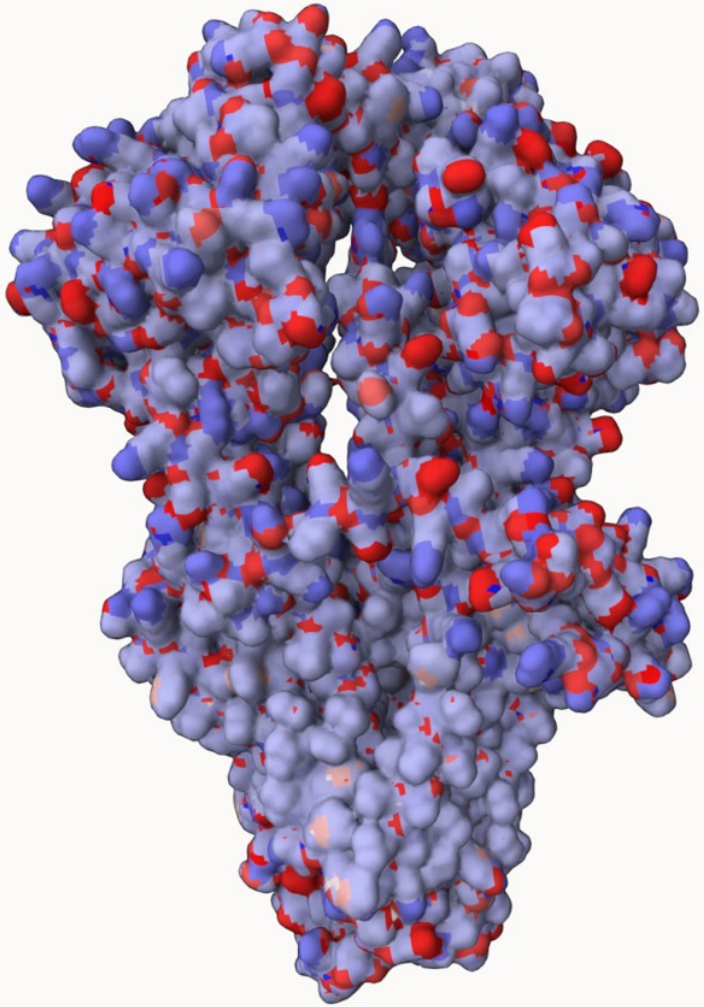


P-glycoprotein

Why partial atomic charges?
They show the chemical properties of the predicted structures

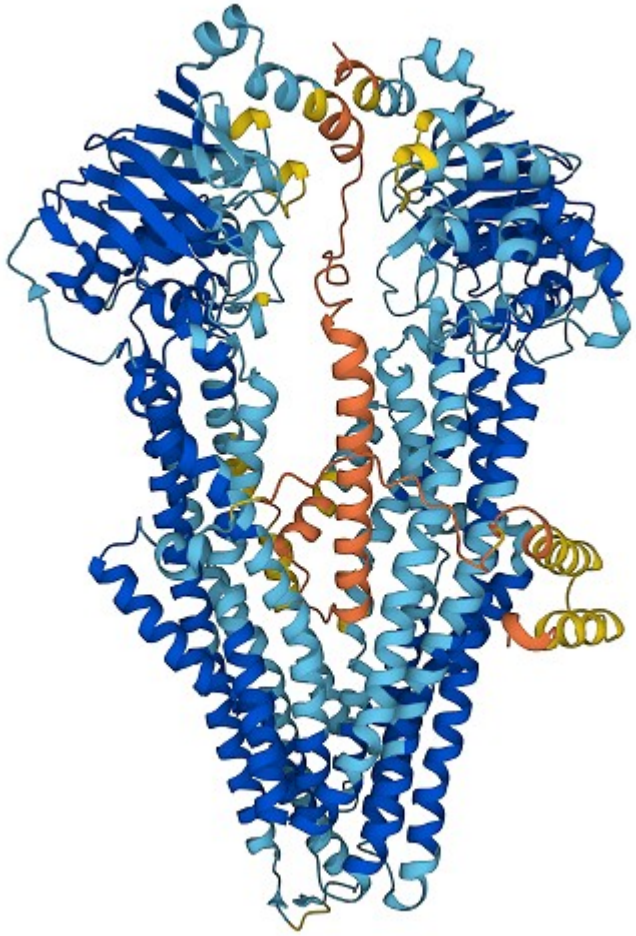


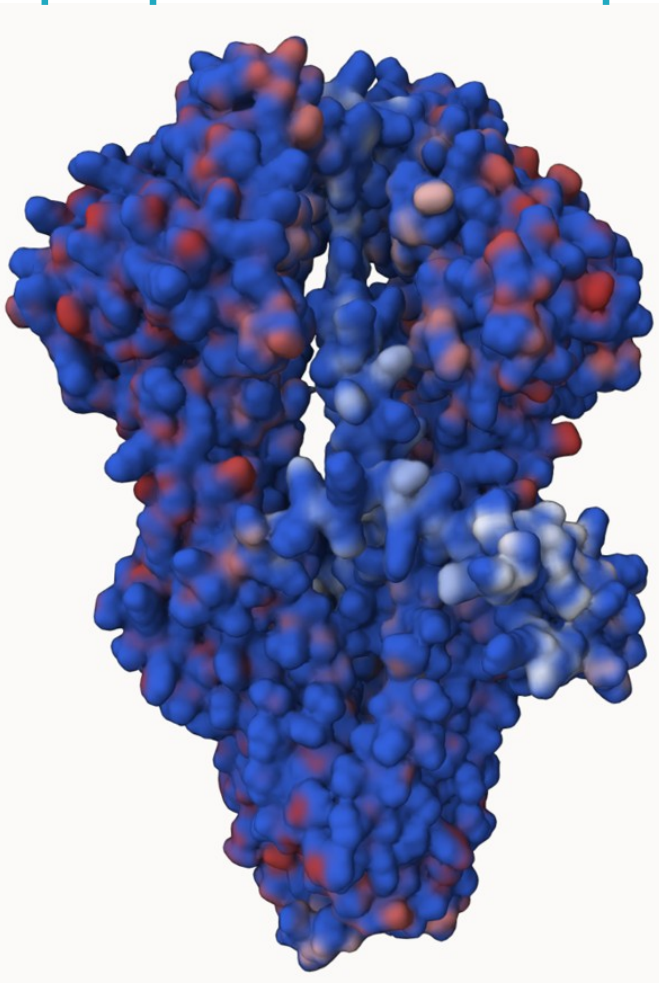


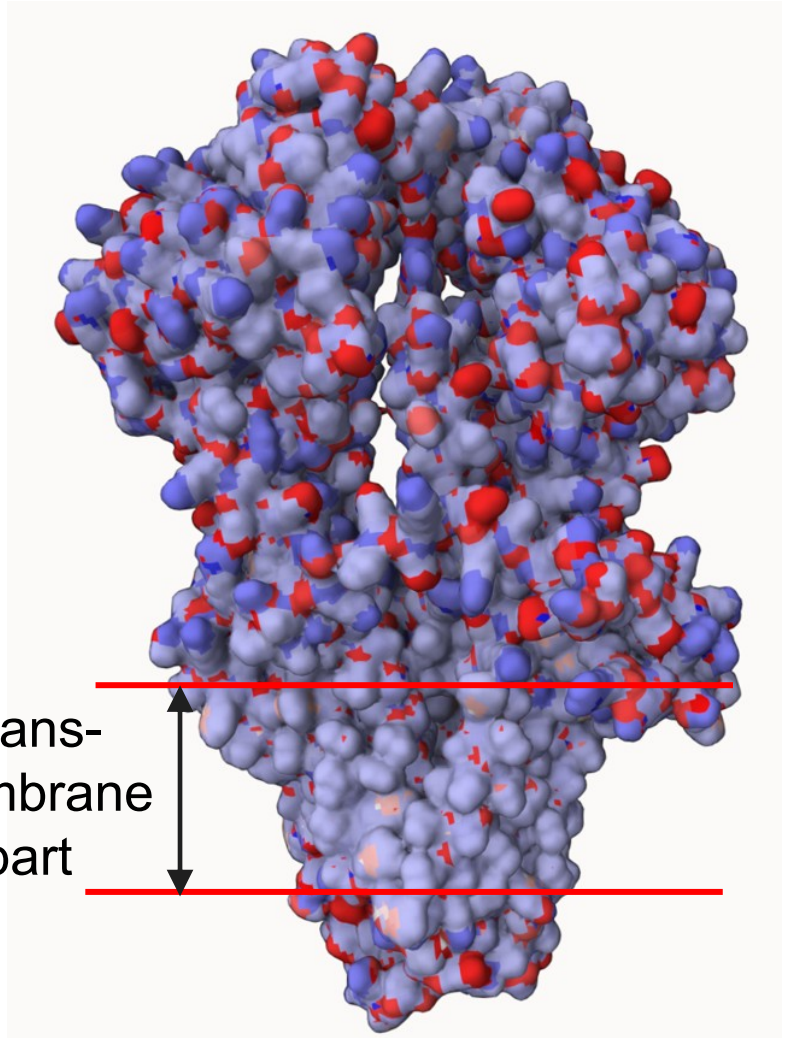


P-glycoprotein

Why partial atomic charges?
They show the chemical properties of the predicted structures



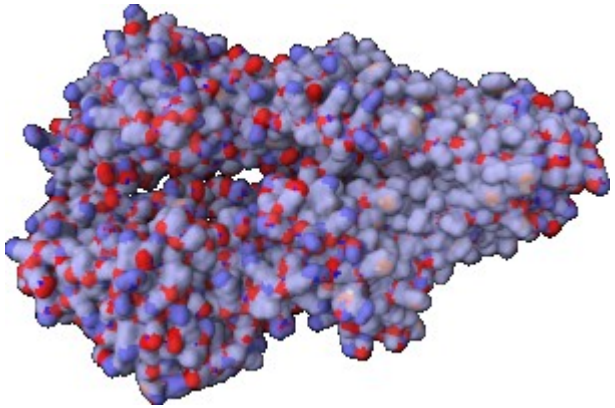


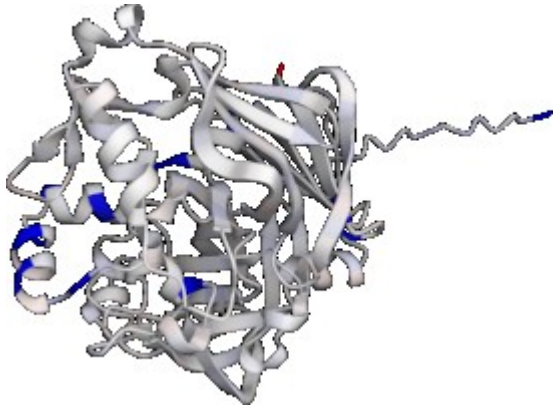


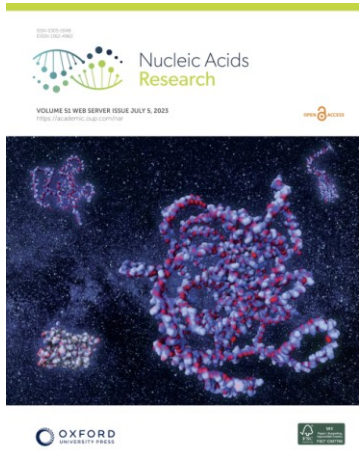
P-glycoprotein

αCharges: Partial atomic charges for AlphaFold structures

- **Computes charges for AlphaFold2 structures from AlphaFoldDB**
- **Method:** SQE+qp, parameterized for (B3LYP/6-31G*/NPA)
- **Inputs:** UniProt ID of AlphaFoldDB molecules
- **Outputs:** plain text, mmCIF, PQR
- **Visualization:** Mol*
- **Web page:** https://alphacharges.ncbr.muni.cz/

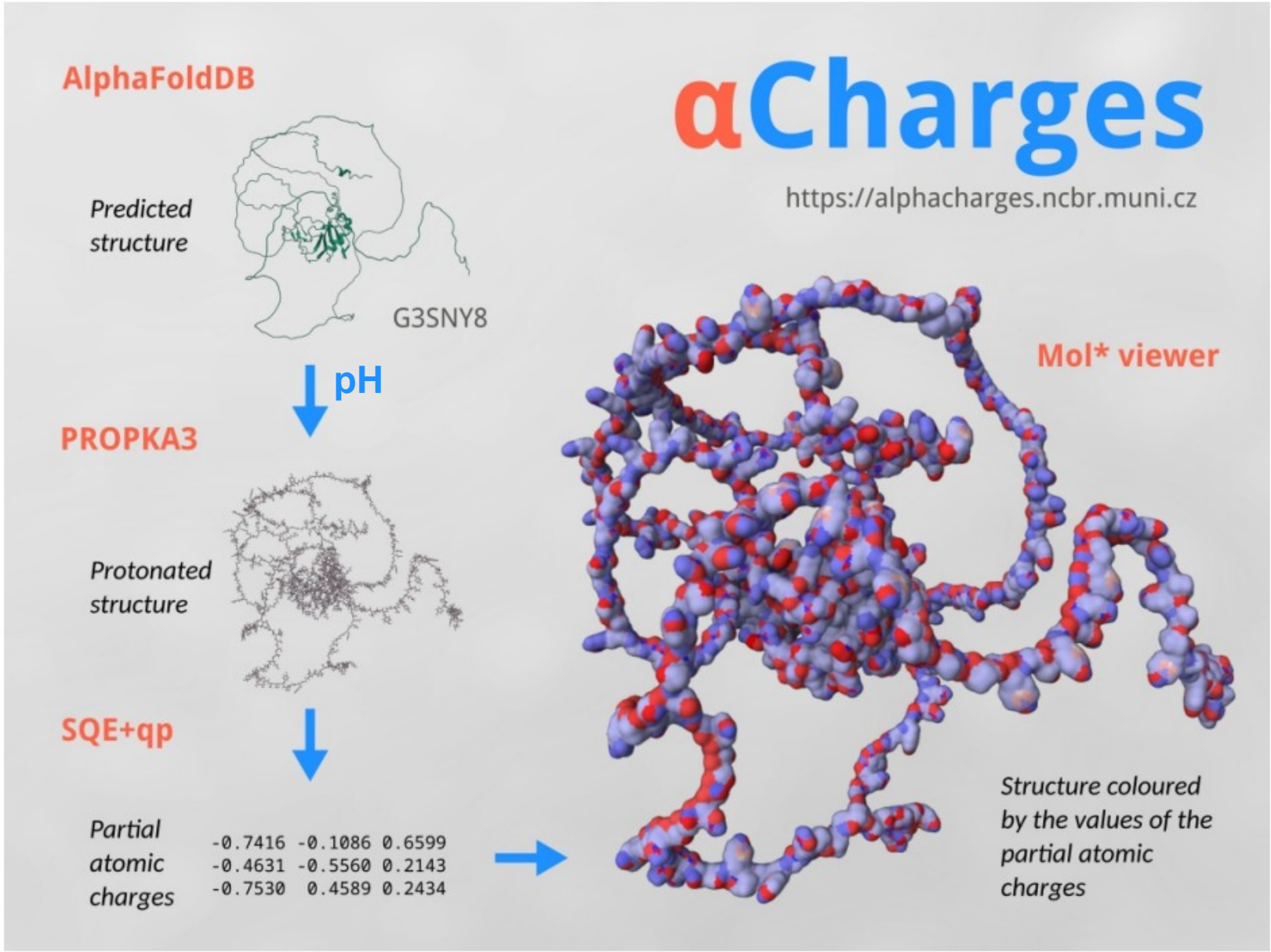






Schindler O., Berka K., Cantara A., Křenek A., Tichý D., Raček T., Svobodová R, 2023. *αCharges: Partial atomic charges for AlphaFold structures in high quality*. **Nucleic acids research**, 51(W1), W11-W16.

αCharges: Partial atomic charges for AlphaFold structures



αCharges

AlphaCharges (**αCharges**) is a web application for the calculation of partial atomic charges on protein structures predicted by the AlphaFold2 algorithm and deposited in the AlphaFoldDB database. The charges are computed by the SQE+qp empirical method, which quality is comparable to quantum mechanical charge calculation approaches (specifically, it is parameterized using B3LYP/6-31G*/NPA quantum mechanical charges). Before computation of the charges, **αCharges** protonates the input protein structures by PROPKA3. The details about the methodology and usage are described in the manual. This website is free and open to all users and there is no login requirement. Source codes are freely available at GitHub.

UniProt code:

e.g., P34712, L8BU87

Calculate charges | Setup calculation

αCharges – Calculation settings

UniProt code: P34712

Protonate in pH:

7.2

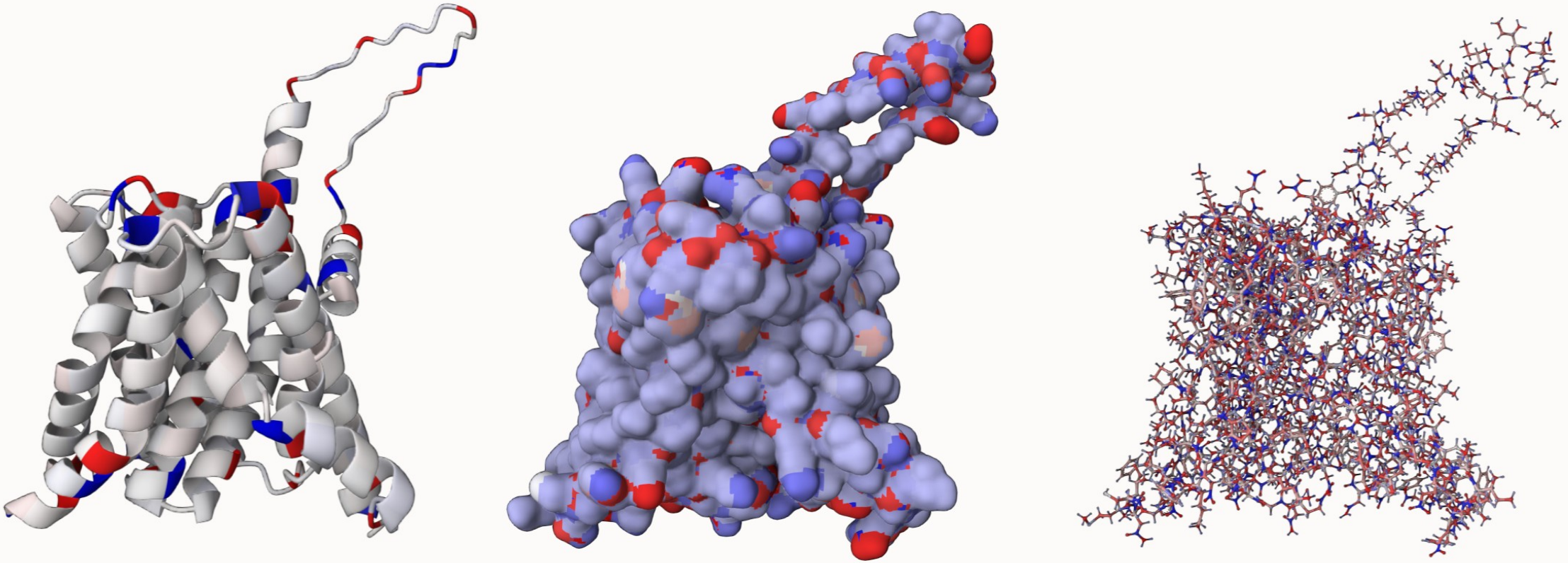
AlphaFold prediction version:

4

Calculate charges

Back to main page

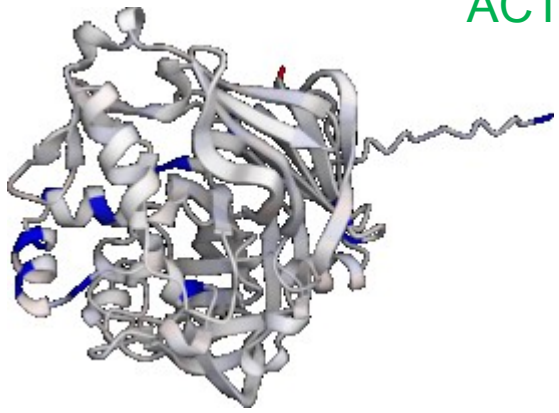
αCharges: visualization



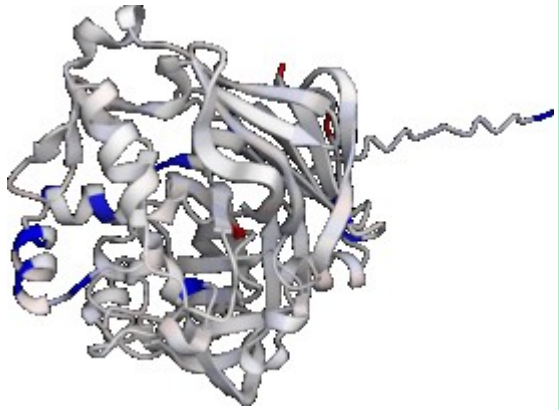
Sehnal D., Bittrich S., Deshpande M., Svobodová R., Berka K., Bazgier V., ... & Rose A. S. (2021). *Mol* Viewer: modern web app for 3D visualization and analysis of large biomolecular structures*. **Nucleic Acids Research**, *49*(W1), W431-W437.

Examples: Pepsin in different pH values

ACTIVE

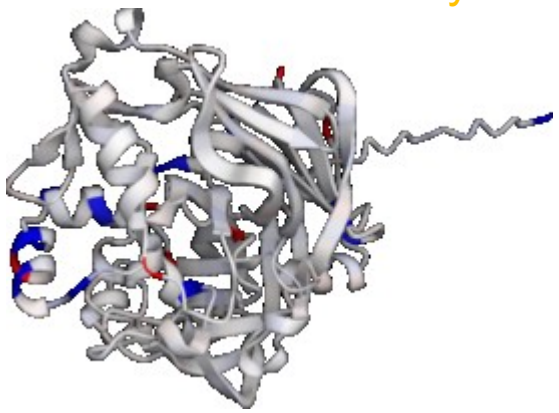


pH 1

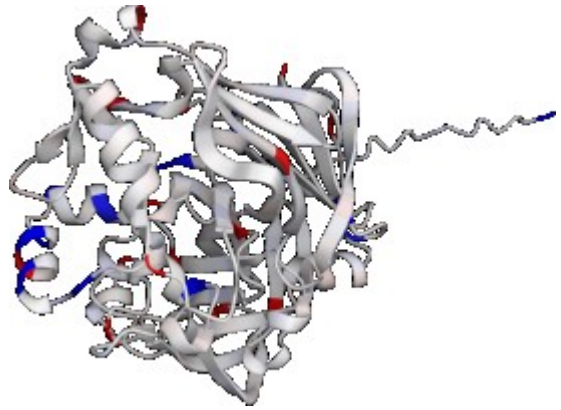


pH 2

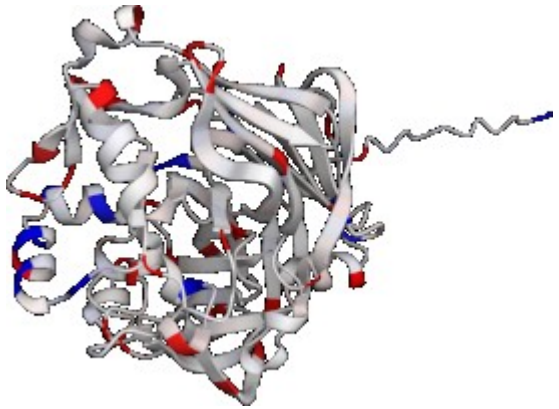
activity decrease



pH 3

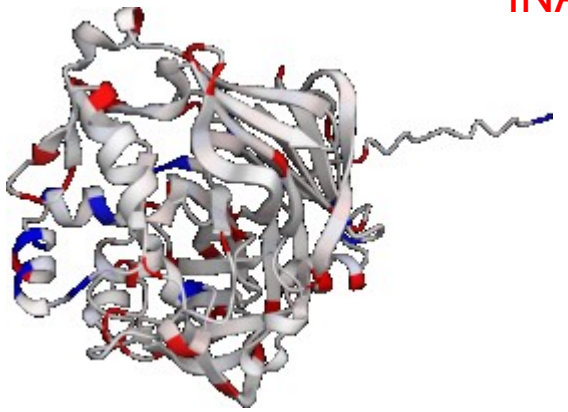


pH 4

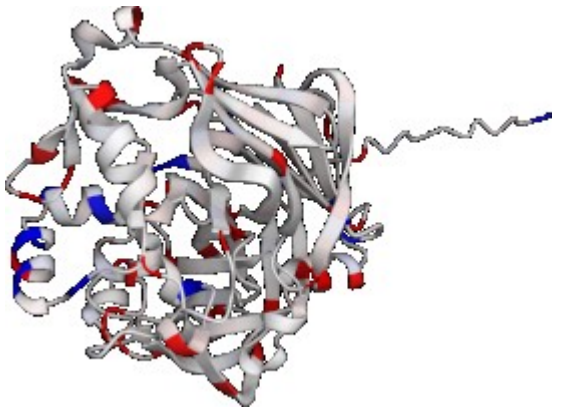


pH 5

INACTIVE

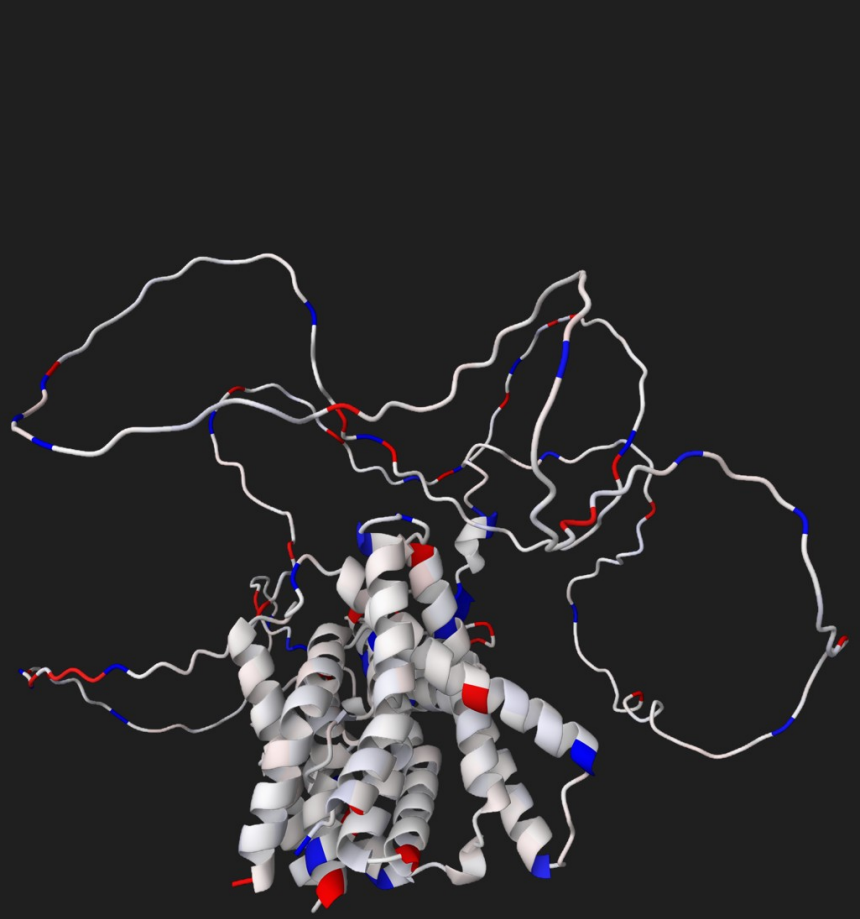


pH 6

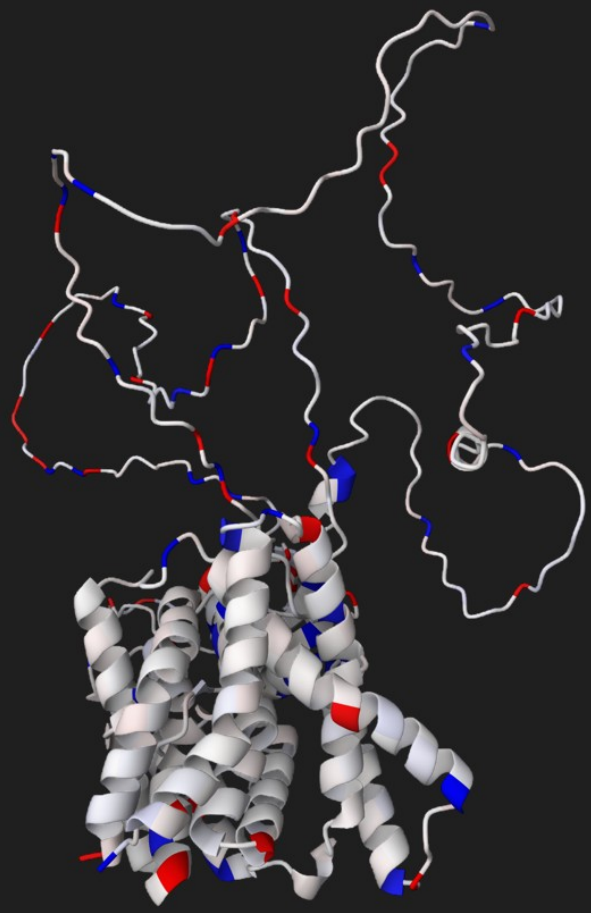


pH 7

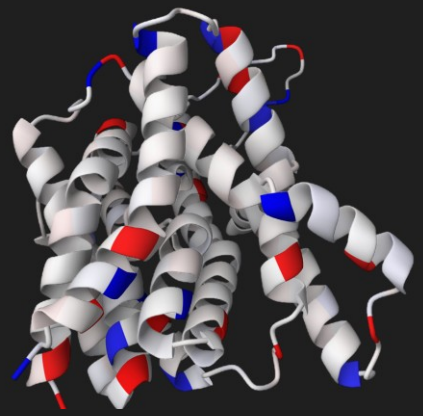
Examples: PIN proteins



PIN3

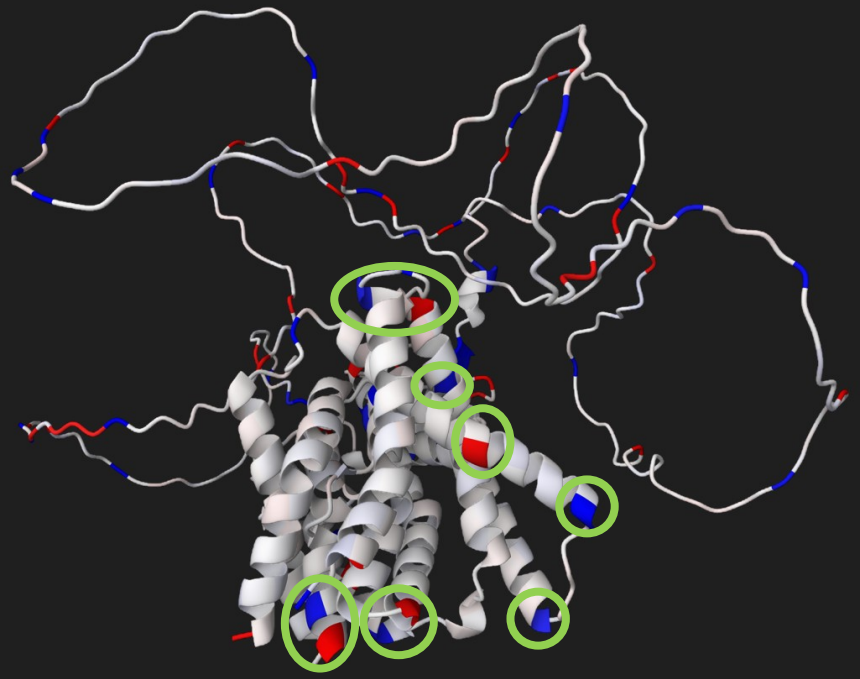


PIN7

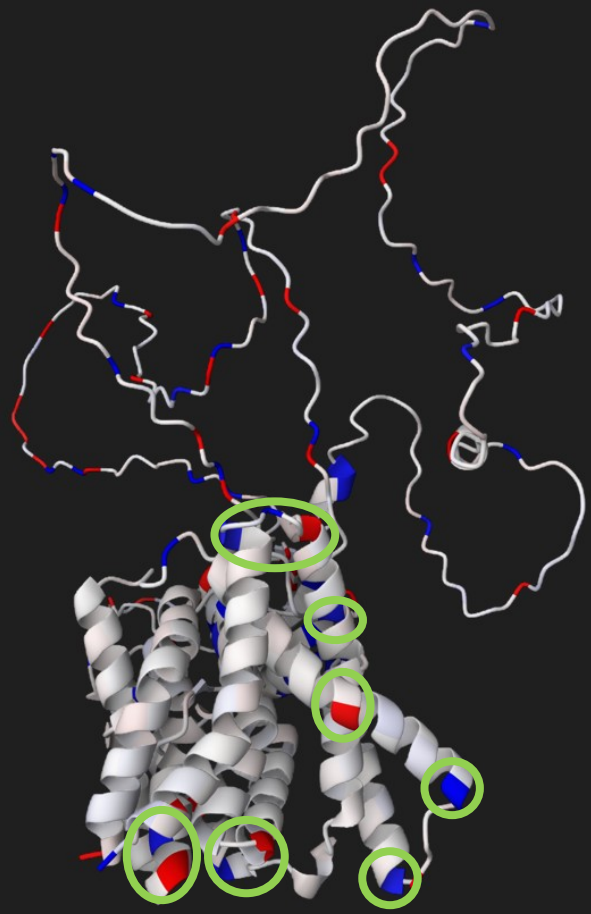


PIN5

Examples: PIN proteins

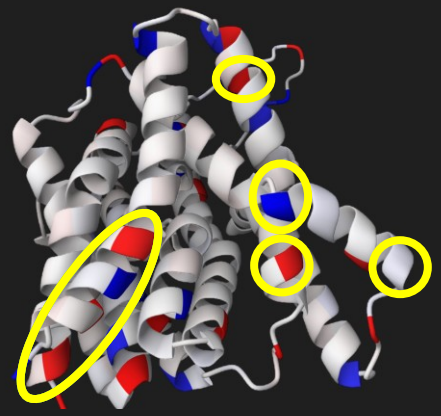


PIN3



PIN7

Legend:
Similar charges
Different charges



PIN5