



AlphaCharges

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1 Overview

AlphaCharges is an online application to calculate partial atom charges of structures from the AlphaFold Database.

1.1 Main Page

The main page offers the possibility to upload the chosen structure (as an UNIPROT code from the AlphaFold Database) and to setup the desired pH through the "Setup calculation" button. Clicking on "Calculate charges" will redirect you to the result page.

UniProt code:	pH:
<input type="text"/>	<input type="text" value="7.2"/>
<input type="button" value="Calculate charges"/>	<input type="button" value="Setup calculation"/>
<input type="button" value="Calculate charges"/>	

1.2 Calculation Results

The results page includes a series of information and visualization options. On top of the screen, Structure code, Number of Atoms, chosen pH and Calculation time are shown.

AlphaCharges - Calculation results

UniProt code: P02730

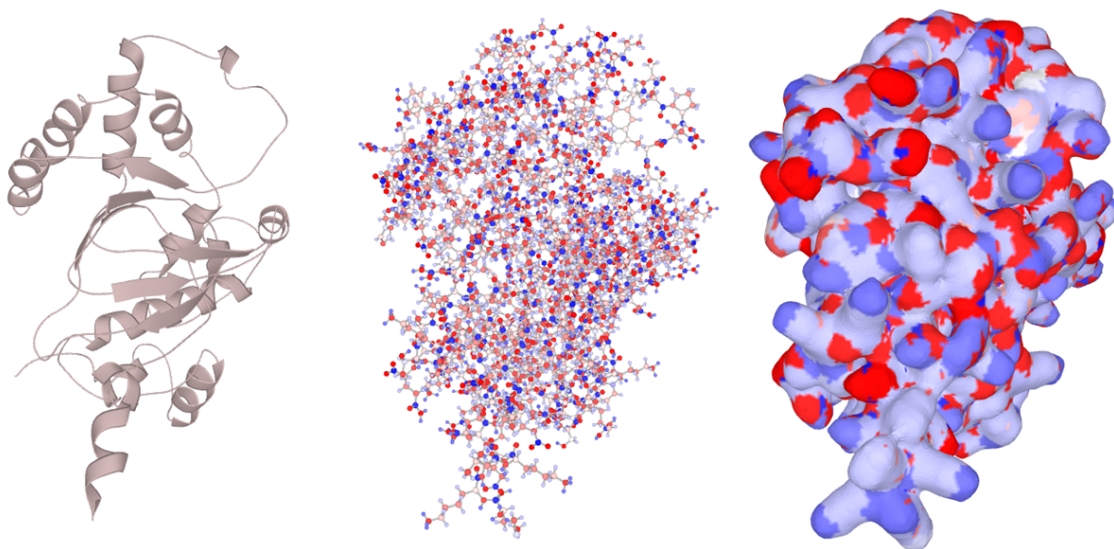
Number of atoms: 14466

pH: 7.2

Calculation time: 36.06 seconds

1.2.1 Visualization Modes

Following, the user can switch between different type of views, visualising the chosen structure as “Cartoon” (first figure, where the color of residues is determined by the sum of charges in the atoms) , “Balls and sticks” and “Surface” (the surface of the molecules is colored accordingly to the nearest atoms), colouring the images according to the structure or the relative (where positive and negative charges are colored in blue and red respectively, adjusted on the largest absolute value computed) and absolute charges (which gives comparable colors between different structures).



1.2.2 Downloading Data

The “Download charges” button allow the user to download a zip file containing charges in four formats: plain text, PDB, CIF and PQR.

2 Bug Reporting

If you encounter an error, please send a report to Ondřej Schindler. Thank you!