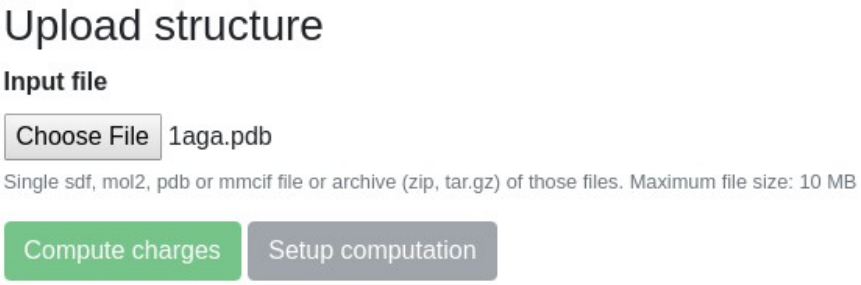
Atomic Charge Calculator II

Atomic Charge Calculator II (ACC II) is a web application providing a user interface for computation of partial atomic charges. The application consists of three main pages – main, introductory one, computation setup and visualization of the results.

Main page

Main page offers a possibility to upload your own structure (in one of the supported formats: SDF, PDB, Mol2, and mmCIF).



Clicking on “Compute charges” button will automatically select the most appropriate method, executes the computation and redirects to the Results page. “Setup computation” can be used for manually selecting the method and parameters.

Input files notes

PDB, mmCIF: When file contains multiple models, only the first one is used for computation. All atoms (including HETATM) atoms are considered.

SDF: Both MOL V2000 and V3000 are supported.

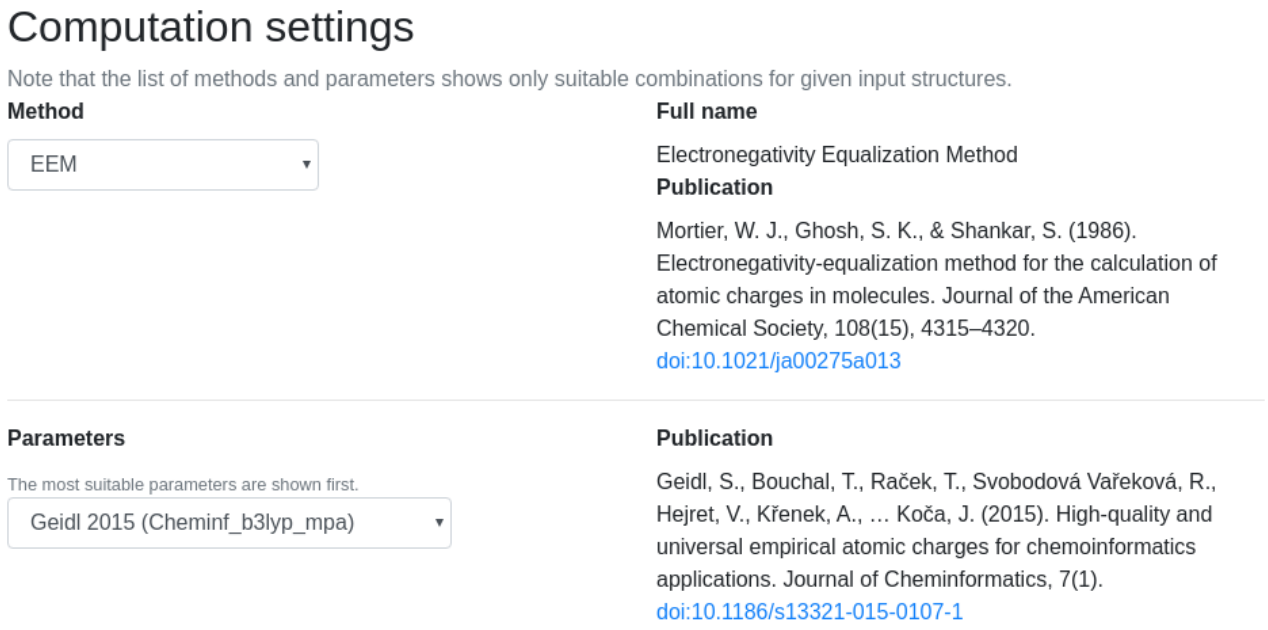
Input file can be zipped.

A size of input file is limited to 10 MB.

Computation settings

Based on the molecules provided, methods (and parameters) that are suitable for *all* structures are displayed. Parameter set is suitable for a given input if it covers all the atomic types contained in input files. Method is suitable if it has at least one suitable set of parameters; or uses no parameters. Additionally, some methods might be omitted if input contains at least one big molecule (i.e., having over 20,000 atoms).

All the methods and parameters have direct links to the original publications. Theoretical background of the methods is summarized here. For easy identification, the name of the parameters used in a publication is enclosed in the brackets.



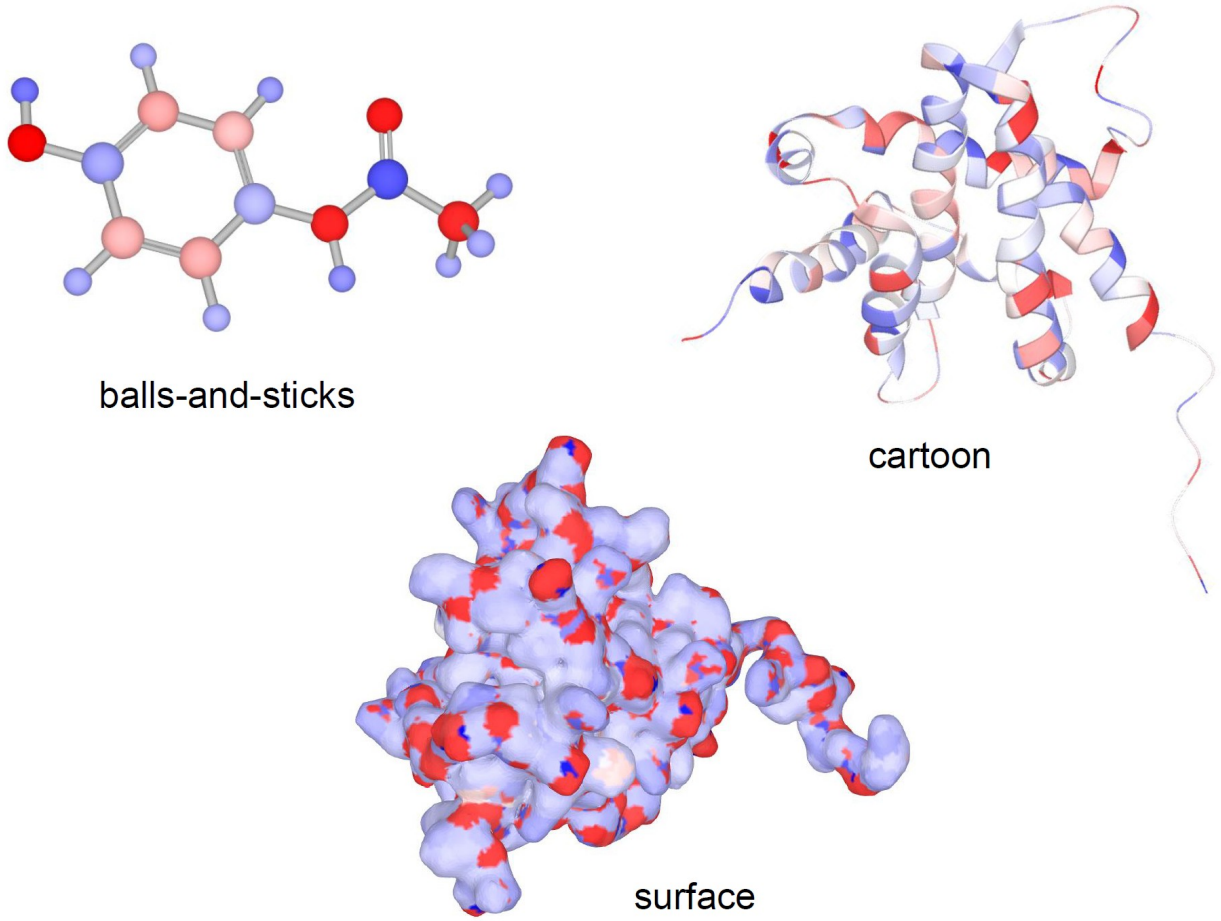
Results

Final page features visualization of the charges and possibility to download calculated charges. At the top it states which method and parameters were used (useful when automatic selection was used).

When multiple structures were provided user can switch between those using the select box.

Visualization modes

ACC II features fast LiteMol viewer to visualize calculated charges. There are three standard modes user can select – balls-and-sticks, cartoon, and surface – see figure:



Default is determined from the structure itself.

Note that to visualize mmCIF files, they must contain _atom_sites category.

Coloring options

Atoms are colored by charges by default – red for negative charges, blue for positive ones. When relative coloring is selected, the range for the colors is adjusted automatically based on the largest absolute value of a charge computed. To have comparable colors between different structures, absolute coloring should be used instead.

In cartoon mode, the color of individual residue is determined according to the sum of charges of all the comprised atoms.

In surface mode, the point on the surface of the molecule is colored according to the nearest atom.

Alternatively, coloring by charges can be disabled – colors are selected based on the elements.

Downloading data

The charges are available in three formats – plain text, Mol2 and PQR. Plain text is present for all the inputs, PQR when input contains structures with chain specification (most likely protein) and Mol2 otherwise (small molecules).