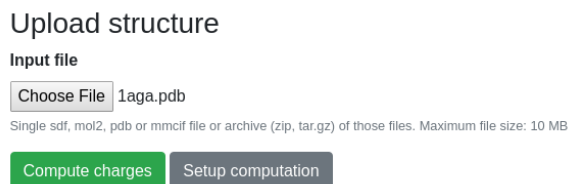# Atomic Charge Calculator II

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

Main page

The 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.

Upload structure

Input file

Choose File   1aga.pdb

Single sdf, mol2, pdb or mmcif file or archive (zip, tar.gz) of those files. Maximum file size: 10 MB

Compute charges   Setup computation

Input files notes

Input file can be zipped. A size of input file is limited to 10 MB.

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.

Formal charges, if present, are read from an input file as well. Their sum is used as a total molecular charge, which is used by some methods (ABEEM, EEM, EQeq, Eqeq+C, QEq, SFKEEM, SMP/QEq, TSEF).

Computation settings

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

Automatic selection works in a same manner. After initial filtering described above, 3D methods are preferred over the 2D ones. When input contains protein structures, parameters for proteins are used (this is the case for EEM having the most parameters to choose from).

Computation settings

Note that the list of methods and parameters shows only suitable combinations for given input structures.

Method	Full name
EEM ▾	Electronegativity Equalization Method

Publication

Mortier, W. J., Ghosh, S. K., & Shankar, S. (1986). Electronegativity-equalization method for the calculation of atomic charges in molecules. Journal of the American Chemical Society, 108(15), 4315–4320. doi:10.1021/ja00275a013

Parameters	Publication
The most suitable parameters are shown first.	Ionescu, C.-M., Geidl, S., Svobodová Vařeková, R., & Koča, J. (2013). Rapid Calculation of Accurate Atomic Charges for Proteins via the Electronegativity Equalization Method. Journal of Chemical Information and Modeling, 53(10), 2548–2558. doi:10.1021/ci400448n
Ionescu 2013 (EX-NPA_6-31Gd_gas) ▾	

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

Results

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

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

Computation results

Method: EEM
Parameters: Ionescu 2013 (EX-NPA_6-31Gd_gas)

Structure:

| 1AGA ▾ |
|---|

Visualization modes

ACC II features fast LiteMol viewer to visualize calculated charges. There are three standard modes the user can select – balls-and-sticks, cartoon, and surface – see example (1F16):

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.
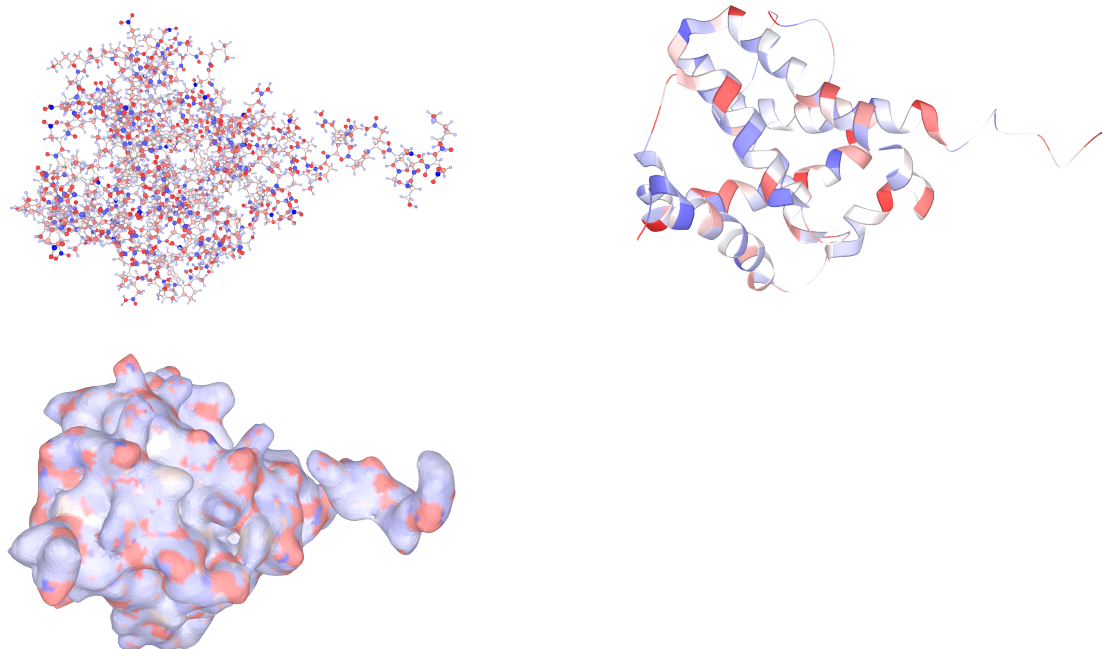
Downloading data

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).

Browser compatibility

OS	Version	Chrome	Firefox	Edge	Safari
Linux	Fedora 31	80	73	n/a	n/a
Windows	10 (1909)	80	73	44	n/a
macOS	?	?	?	?	?

Bug reporting

If you encounter an error, please send a report to krab1k@mail.muni.cz. Thank you!