NAME

density−fitness − Calculates per-residue electron density scores real-space R, real-space correlation coefficient, EDIAm, and OPIA

SYNOPSIS

density−fitness [OPTION] <mtz-file> <coordinates-file> [output]

density−fitness [OPTION] --hklin=<mtz-file> --xyzin=<coordinates-file> [--output=<output>]

density−fitness [OPTION] --fomap=<fo-map-file> --dfmap=<df-map-file> --reslo=<low-resolution> --reshi=<high-resolution> --xyzin=<input [--output=<output>]

DESCRIPTION

The program density-fitness calculates electron density metrics, for main- (includes Cβ atom) and side-chain atoms of individual residues.

For this calculation, the program uses the structure model in either PDB or mmCIF format and the electron density from the 2mFo-DFc and mFo-DFc maps. If these maps are not readily available, the MTZ file and model can be used to calculate maps clipper. Density-fitness support both X-ray and electron diffraction data.

This program is essentially a reimplementation of *edstats*, a program available from the CCP4 suite. However, the output now contains only the RSR, SRSR and RSCC fields as in *edstats* with the addition of EDIAm and OPIA and no longer requires pre-calculated map coefficients.

The real-space R factor (RSR) is defined (Brändén & Jones, 1990; Jones et al., 1991) as:

$$RSR = \Sigma |\rho obs - \rho calc| / \Sigma |\rho obs + \rho calc|$$

The SRSR is the estimated sigma for RSR.

The real-space correlation coefficient (RSCC) is defined as:

$$RSCC = cov(\rho obs, \rho calc) / sqrt(var(\rho obs)\ var(\rho calc))$$

where cov(.,.) and var(.) are the sample covariance and variance (i.e. calculated with respect to the sample means of ρobs and ρcalc).

The EDIAm score is a per-residue score based on the atomic EDIA value and the OPIA score gives the percentage of atoms in the residue with EDIA score is above 0.8.

OPTIONS

When using MTZ files, the input and output files do not need the option flag. If no output file is given, the result is printed to *stdout*.

When using map files, the resolution **must** be specified using the *reshi* and *reslo* options.

--xyzin The coordinates file in either PDB or mmCIF format. This file may be compressed with gzip or bzip2. **--fomap** and **--dfmap** The *2mFo-DFc* and *mFo-DFc* map files respectively. Both are required and if these are specified, the resolution **must** also be specified.

--reslo and **--reshi**
The low and high resolution for the specified map files.

--hklin The MTZ file. If this option is specified, the maps will be calculated using the information in this file.

--sampling-rate
The sampling rate to use when creating maps. Default is 1.5.

--recalc
By default the maps are read from the MTZ file, but you can also opt to recalculate the maps, e.g. when the structure no longer corresponds to the structure used to calculate the maps in the MTZ file.

--aniso-scaling
Accepted values for this option are *observed* and *calculated* or *none*. Used when recalculating maps.

--no-bulk
When specified, a bulk solvent mask is not used in recalculating the maps.

--components (or **--compounds**)
Specify the path of the CCD file components.cif. By default the one installed by libcifpp is used, use this option to override this default.

--extra-compounds
A file containing information for residues in this specific target. This file may be in either CCD or CCP4 monomer library format.

--mmcif-dictionary
Specify the path to the mmcif pdbx dictionary file. The default is to use the dictionary installed by libcifpp, use this option to override this default.

--no-validate
Omit the validation of the input mmCIF file. This will force output even in case the input file contains errors.

--electron-scattering
Use electron scattering factors instead of X-ray scattering factors.

--use-auth-ids
By default, when reading mmCIF files, the label_xxx_id is used in the edstats output. Use this flag to force output with the auth_xxx_ids.

--output-format
By default a JSON file is written, unless the filename ends with .eds. Use this option to force output in *edstats* or *json* format.

--verbose,-V
Be more verbose, useful to diagnose validation errors.

REFERENCES

References:

Statistical quality indicators for electron-density maps
Tickle, I. J. (2012). Acta Cryst. D68, 454-467. DOI: 10.1107/S0907444911035918

Estimating Electron Density Support for Individual Atoms and Molecular Fragments in X-ray Structures
Agnes Meyder, Eva Nittinger, Gudrun Lange, Robert Klein, and Matthias Rarey Journal of Chemical Information and Modeling 2017 57 (10), 2437-2447 DOI: 10.1021/acs.jcim.7b00391

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REPORTING BUGS

Report bugs at https://github.com/PDB-REDO/density-fitness/issues