

NAME

tortoise – Calculate ramachandran z-scores

SYNOPSIS

tortoise [OPTION] input [output]

DESCRIPTION

Tortoise validates protein structure models by checking the Ramachandran plot and side-chain rotamer distributions. Quality Z-scores are given at the residue level and at the model level (ramachandran-z and torsions-z). Higher scores are better. To compare models or to describe the reliability of the model Z-scores jackknife- based standard deviations are also reported (ramachandran-jackknife-sd and torsion-jackknife-sd).

OPTIONS

The input file can be either mmCIF or PDB format and the file may be gzip or bzip2 compressed.

The output is a json file, if no file name is specified the output is written to *stdout*.

--dict=<file>

Specify a dictionary file containing restraints for residues specific to this file.

--log=<file>

Write a log with diagnostic information to this file.

REFERENCES

References:

Sobolev et al.

A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry, Structure (2020), DOI: <https://doi.org/10.1016/j.str.2020.08.005>

Van Beusekom et al.

Homology-based loop modeling yields more complete crystallographic protein structures, IUCrJ (2018), DOI: <https://doi.org/10.1107/S2052252518010552>

Hooft et al.

Objectively judging the quality of a protein structure from a Ramachandran plot, CABIOS (1993), DOI: <https://doi.org/10.1093/bioinformatics/13.4.425>

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REPORTING BUGS

Report bugs at <https://github.com/PDB-REDO/tortoise/issues>