Resource Summary Report

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NRG-CING

RRID:SCR_006079
Type: Tool

Proper Citation

NRG-CING (RRID:SCR_006079)

Resource Information

URL: http://nmr.cmbi.ru.nl/NRG-CING/HTML/index.html

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Description: NRG-CING presents a complete validation report for all 9,000+ wwPDB NMR entries including remediated experimental data such as chemical shifts from BMRB and restraints from NRG . These CING reports are compiled from internal analyses and those by CCPN, DSSP, PROCHECK-NMR/Aqua, ShiftX, Talos+, Vasco, Wattos, and WHAT_CHECK. The NRG-CING website is a collection of CING reports that has been pre-calculated for all PDB files solved by NMR. (See website for more information on CING.) In case the underlying experimental data is available, these have been cleaned up and made syntactically and semantically correct and homogeneous. For many macromolecular NMR ensembles from the Protein Data Bank (PDB) the experiment-based restraint lists used in the structure calculation are accessible, while other experimental data, mainly chemical shift values, are often available from the BioMagResBank. Assessment of the quality of the structural result is paramount to their usage and a combined, integrated repository of both input data and structural results greatly facilitates such an analysis. In addition, the accuracy and precision of the coordinates in these macromolecular NMR ensembles can be improved by recalculations using the available experimental data and present-day software with improved protocols and force fields. Such efforts, however, generally fail on over half of all deposited structures due to the syntactic and semantic heterogeneity of the data and the wide variety of formats used for their deposition. We have combined the cleaned-up restraints information from the NMR Restraints Grid (NRG) database with available chemical shifts from the BioMagResBank in the weekly updated NRG-CING database. Eleven programs, in addition to CING itself, have been included in the NRG-CING production pipeline to arrive at validation reports that list for each entry the potential inconsistencies between the coordinates and the available restraint and chemical shift data. The longitudinal validation of this data yielded a set of indicators that can be used to judge the quality of every macromolecular structure solved with NMR. The cleaned up NMR experimental datasets and

the validation reports are freely available.

Abbreviations: NRG-CING

Resource Type: database, data or information resource

Defining Citation: PMID:22139937

Keywords: macromolecular structure, nmr, macromolecule, restraint, chemical shift, validation report, validation, bio.tools

Funding: Netherlands Organization for Scientific Research (NWO) 700.55.443;
Netherlands Bioinformatics Centre (NBIC) ;
EU FP6 LSHG-CT-2005-018988;
EU FP6 LHSG-CT-2004-512092;
EU FP7 261572;
Brussels Institute for Research and Innovation BB2B 2010-1-12;
NLM LM05799

Availability: Free

Resource Name: NRG-CING

Resource ID: SCR_006079

Alternate IDs: nlx_151486, biotools:nrg-cing

Alternate URLs: https://bio.tools/nrg-cing

Record Creation Time: 20220129T080234+0000

Record Last Update: 20250412T055022+0000

Ratings and Alerts

No rating or validation information has been found for NRG-CING.

No alerts have been found for NRG-CING.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 1 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

Sousa da Silva AW, et al. (2012) ACPYPE - AnteChamber PYthon Parser interfacE. BMC research notes, 5, 367.