Databases and ontologies

ValTrendsDB: bringing Protein Data Bank validation information closer to the user

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Received on February 19, 2019; revised on June 1, 2019; editorial decision on June 21, 2019; accepted on June 28, 2019

Abstract

Summary: Structures in PDB tend to contain errors. This is a very serious issue for authors that rely on such potentially problematic data. The community of structural biologists develops validation methods as countermeasures, which are also included in the PDB deposition system. But how are these validation efforts influencing the structure quality of subsequently published data? Which quality aspects are improving, and which remain problematic? We developed ValTrendsDB, a database that provides the results of an extensive exploratory analysis of relationships between quality criteria, size and metadata of biomacromolecules. Key input data are sourced from PDB. The discovered trends are presented via precomputed information-rich plots. ValTrendsDB also supports the visualization of a set of user-defined structures on top of general quality trends. Therefore, ValTrendsDB enables users to see the quality of structures published by selected author, laboratory or journal, discover quality outliers, etc. ValTrendsDB is updated weekly.

Availability and implementation: Freely accessible at http://ncbr.muni.cz/ValTrendsDB. The web interface was implemented in JavaScript. The database was implemented in C++.

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Supplementary information: Supplementary data are available at Bioinformatics online.

1 Introduction

Biomacromolecular structural data are key results of modern life sciences. Their importance is reinforced by 13 Nobel prizes that were awarded for research on these data (ebi.ac.uk/pdbe/docs/nobel/nobel. html). Most structures of biomacromolecules and their ligands are accessible via the Protein Data Bank (PDB) database (Burley et al., 2018). However, some structures were found to contain serious errors (Rupp, 2012). This discovery showed the importance of the validation of biomacromolecular complexes. The first validation approaches were focused on the geometric properties of standard biomacromolecular residues (i.e. amino acids, nucleotides) (Chen et al., 2010). This validation approach was later extended to validate ligands (Bruno et al., 2004). A step forward in validation was the release of PDB validation reports (Gore et al., 2017) for almost every structure.

A major question is how the validation efforts of the scientific community are influencing the quality of structural data. Our cooperation with the Protein Data Bank in Europe (PDBe) motivated us to ask broader questions: How is the quality of biomacromolecular complexes changing over time? What factors are influencing it? To suggest answers to these questions, we carried out an exploratory analysis of trends between quality criteria, size (e.g. atom count) and the metadata of biomacromolecules (e.g. year of release). Its results can be explored in the novel ValTrendsDB database.

2 Database construction

ValTrendsDB is a database that presents the results of the factor pair relationship analysis. A factor represents a property or a
ValTrendsDB is unique because of the breadth of the analysis whose results it presents. No other similar published analysis contains as many factors, as many data points, or is updated automatically on a weekly basis. That is why another publication that is being worked on will focus on the analysis itself.

The European Bioinformatics Institute, which maintains the PDB, plans to integrate selected data and some of the plots from ValTrendsDB into their new validation pages. Specifically, PDB will use these data to plot charts that will show the relative quality of an entry, as well as embed a few plots that show database-wide trends. The full functionality of ValTrendsDB will, however, remain solely on its website.

Acknowledgements
We would like to thank Sameer Velankar and Oliver Smart (EMBL-EBI UK) for their valuable input on the whole project. We would also like to thank Jiří Rosecký (FI MU) for implementing the first version of the website.

Funding
This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic under the project CEITEC 2020 [grant number LQ1601]; the ELIXIR-EXCELERATE project, which received funding from the European Union’s Horizon 2020 research and innovation programme [grant number 676559]; ELIXIR CZ research infrastructure project including access to computing and storage facilities [grant number LM2015047]; European Regional Development Fund – projects ELIXIR-CZ [grant number CZ.02.1.01/0.0/0.0/16_013/0001777] and RIAT-CZ [grant number ATCZ40]; and the Grant Agency of Masaryk University [grant number MUNI/A/1503/2018 to V.B.].

Conflict of Interest: none declared.

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