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# MotiveValidator: interactive web-based validation of ligand and residue structure in biomolecular complexes

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## ABSTRACT

**Structure validation has become a major issue in the structural biology community, and an essential step is checking the ligand structure. This paper introduces MotiveValidator, a web-based application for the validation of ligands and residues in PDB or PDBx/mmCIF format files provided by the user. Specifically, MotiveValidator is able to evaluate in a straightforward manner whether the ligand or residue being studied has a correct annotation (3-letter code), i.e. if it has the same topology and stereochemistry as the model ligand or residue with this annotation. If not, MotiveValidator explicitly describes the differences. MotiveValidator offers a user-friendly, interactive and platform-independent environment for validating structures obtained by any type of experiment. The results of the validation are presented in both tabular and graphical form, facilitating their interpretation. MotiveValidator can process thousands of ligands or residues in a single validation run that takes no more than a few minutes. MotiveValidator can be used for testing single structures, or the analysis of large sets of ligands or fragments prepared for binding site analysis, docking or virtual screening. MotiveValidator is freely available via the Internet at http://ncbr.muni.cz/MotiveValidator.**

## INTRODUCTION

Validation arose as a major issue in the structural biology community when it became apparent that some published structures contained serious errors (1–6). Various tools for the validation of the protein and nucleic acid 3D structures are well established, such as WHAT_CHECK (7), PROCHECK (8), MolProbity (9) and OOPS (10).

An essential step in the validation process is checking the ligand structure. Ligands are chemical compounds which form a complex with a biomacromolecule (e.g. sugar, drug, heme) and play a key role in its function. The ligands are also the main source of errors in structures (11,12). Nonetheless, ligand validation is a very challenging task (13), because of the high diversity and nontriviality of their structure and the general lack of information about correct structures. Therefore, early validation tools focused on selected types of ligands (PDB-care (14) focused on carbohydrates) and their scope only widened later (ValLigURL (15)). Ligand validation features were recently added to existing software (e.g. Mogul (16), Coot (17)). New tools such as PHENIX (18) were developed to include ligand validation functionality. However, the functionality of some available tools (i.e. ValLigURL, Mogul, Coot, PHENIX) is aimed at the validation of selected properties (atom clashes, bond lengths, bond angles, etc.) or is limited to a selected type of molecules (e.g. PDB-care validates only carbohydrates).

This article presents the web-based application MotiveValidator, which offers a user-friendly, interactive and platform-independent environment for the validation of ligands and residues in PDB (http://www.wwpdb.org/docs.html) or PDBx/mmCIF (19) files provided by the user.

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