

MotiveValidator

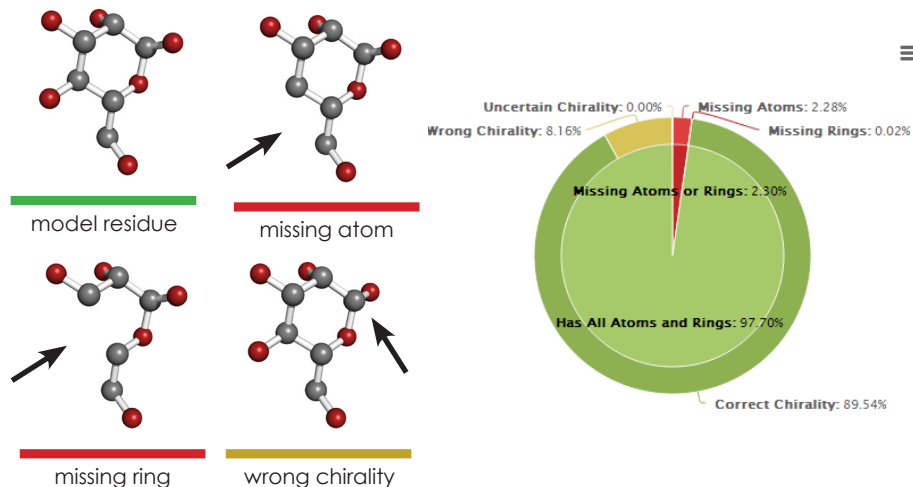
interactive web-based validation of ligand and residue structure in biomolecular complexes

Description:

- Fast and accurate detection of inconsistencies in *ligand* structures in PDB files against wwPDB CCD models.
- Expert *sugar* structure validation.
- User defined *motif/fragment* validation.
- Intuitive and user friendly interface.
- Supports pdb, mol & cif file formats.

MAN [[LigandExpo](#) | [PDB](#) | [MOL](#)] [$C_6H_{12}O_6$ | alpha-D-mannose] [Chiral Atoms (5): C1, C2, C3, C4, C5] [Experimental Coordinates]
5490 motifs in 1282 structures, 11 (0.20%) not processed, 137 warnings

Summary			With All Atoms and Rings						
Missing Atoms or Rings			5364 (97.70%)						
Rings	Only Atoms	Different Naming	Correct Chirality	Wrong Chirality	Planar Warn.	Uncertain Chirality	Substitutions	Foreign	Different Naming
1 (0.02%)	125 (2.28%)	1 (0.02%)	4916 (89.54%)	448 (8.16%)	0 (0.00%)	0 (0.00%)	19 (0.35%)	4984 (90.78%)	3 (0.05%)



<http://ncbr.muni.cz/MotiveValidator>

[1] Vařeková, R.S., et al., (2014) MotiveValidator: interactive web-based validation of ligand and residue structure in biomolecular complexes. *Nucleic Acids Res.*, 42, W227–33, doi: 10.1093/nar/gku426.

MotiveValidator

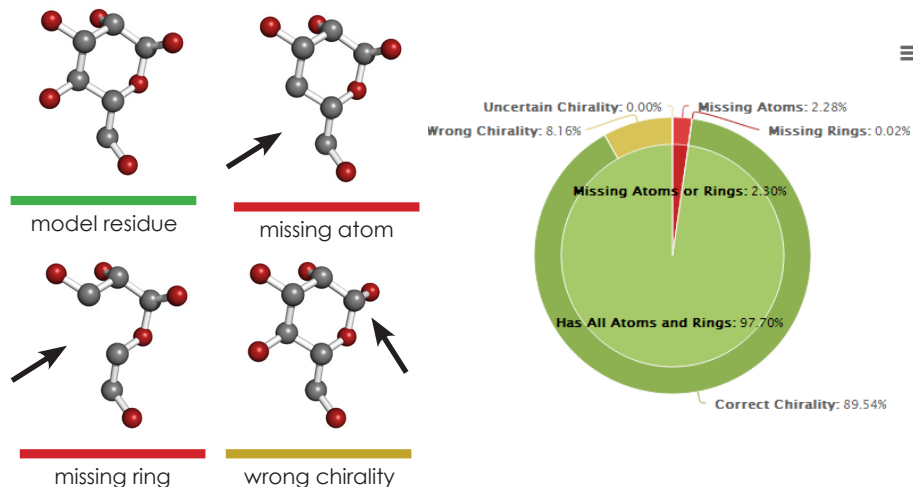
interactive web-based validation of ligand and residue structure in biomolecular complexes

Description:

- Fast and accurate detection of inconsistencies in *ligand* structures in PDB files against wwPDB CCD models.
- Expert *sugar* structure validation.
- User defined *motif/fragment* validation.
- Intuitive and user friendly interface.
- Supports pdb, mol & cif file formats.

MAN [[LigandExpo](#) | [PDB](#) | [MOL](#)] [$C_6H_{12}O_6$ | alpha-D-mannose] [Chiral Atoms (5): C1, C2, C3, C4, C5] [Experimental Coordinates]
5490 motifs in 1282 structures, 11 (0.20%) not processed, 137 warnings

Summary			With All Atoms and Rings						
Missing Atoms or Rings			5364 (97.70%)						
Rings	Only Atoms	Different Naming	Correct Chirality	Wrong Chirality	Planar Warn.	Uncertain Chirality	Substitutions	Foreign	Different Naming
1 (0.02%)	125 (2.28%)	1 (0.02%)	4916 (89.54%)	448 (8.16%)	0 (0.00%)	0 (0.00%)	19 (0.35%)	4984 (90.78%)	3 (0.05%)



<http://ncbr.muni.cz/MotiveValidator>

[1] Vařeková, R.S., et al., (2014) MotiveValidator: interactive web-based validation of ligand and residue structure in biomolecular complexes. *Nucleic Acids Res.*, 42, W227–33, doi: 10.1093/nar/gku426.