MotiveValidator

Validate ligand and residue structure in biomolecular complexes.

MotiveValidator is a platform for a set of applications designed to help you determine whether a residue or a ligand in a biomolecule or biomolecular complex is structurally complete and correctly annotated according to its models stored in the **wwPDB** chemical component dictionary.

The applicat Get oriented... rm cover all residues and ligands defined in the **wwPDB** chemical component dictionary, a ay specify your own model residue if it is not available in **LigandExpo**.

Quick Help | **Residue Validation** | **Sugar Validation** | **Motif/Fragment Validation** | Command Line Version

- Click on each of the application tabs to read about the functionality of a specific **MotiveValidator** application, and upload the structures you wish to study. If you do not have any input PDB or PDBx/mmCIF files ready or are unsure regarding what the input files can look like, just view the results to one of our sample calculations. You will be able to download sample input files from there.
- Note that some of the applications work with the structure of entire biomolecules, whereas other applications work with fragments of these structures.
- Once your calculation is complete, you will be redirected to a results page, where you will be able to analyze your results in detail, both statistically and visually.
- You will be provided with a link to your results page, so that you can return, analyze or download your results later. The results page address is not publicly visible.
- For a step-by-step guide about how to work with MotiveValidator and how to analyze your results, see the Manual. Should you have any further questions or comments, feel free to contact us at david.sehnal@mail.muni.cz.
- For a quick demo, view the Tutorial and examine the results of our Sample calculations.

Database mirrors last updated 3/27/2014. LigandExpo with 17516 ligands (view all, sugars), PDB with 98900 structures.
Service version 1.0.14.3.27 (change log).

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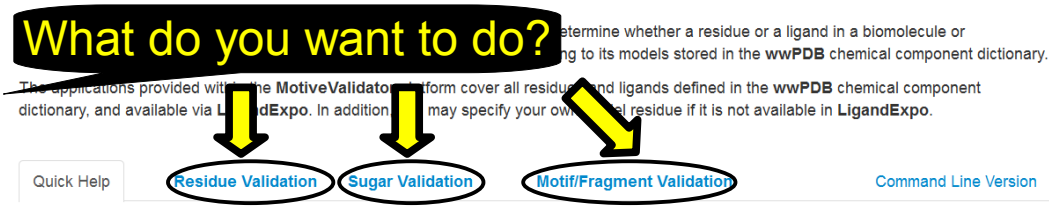

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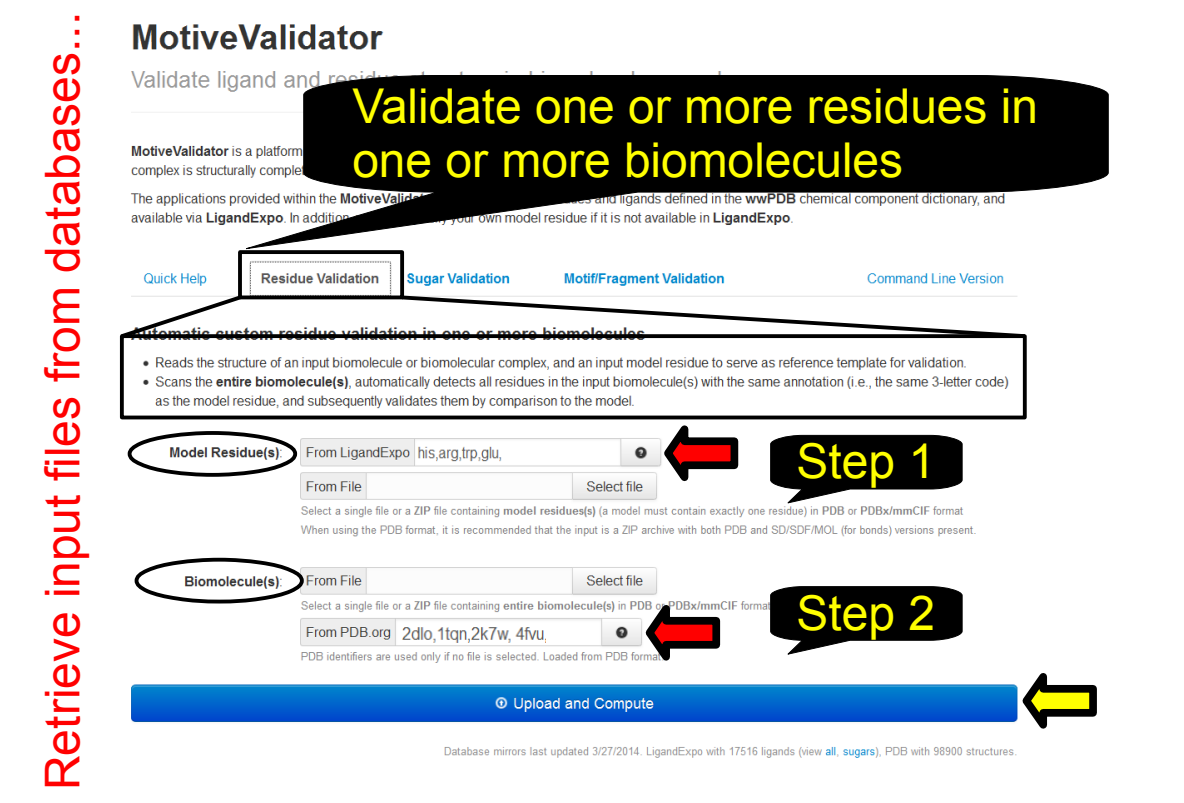
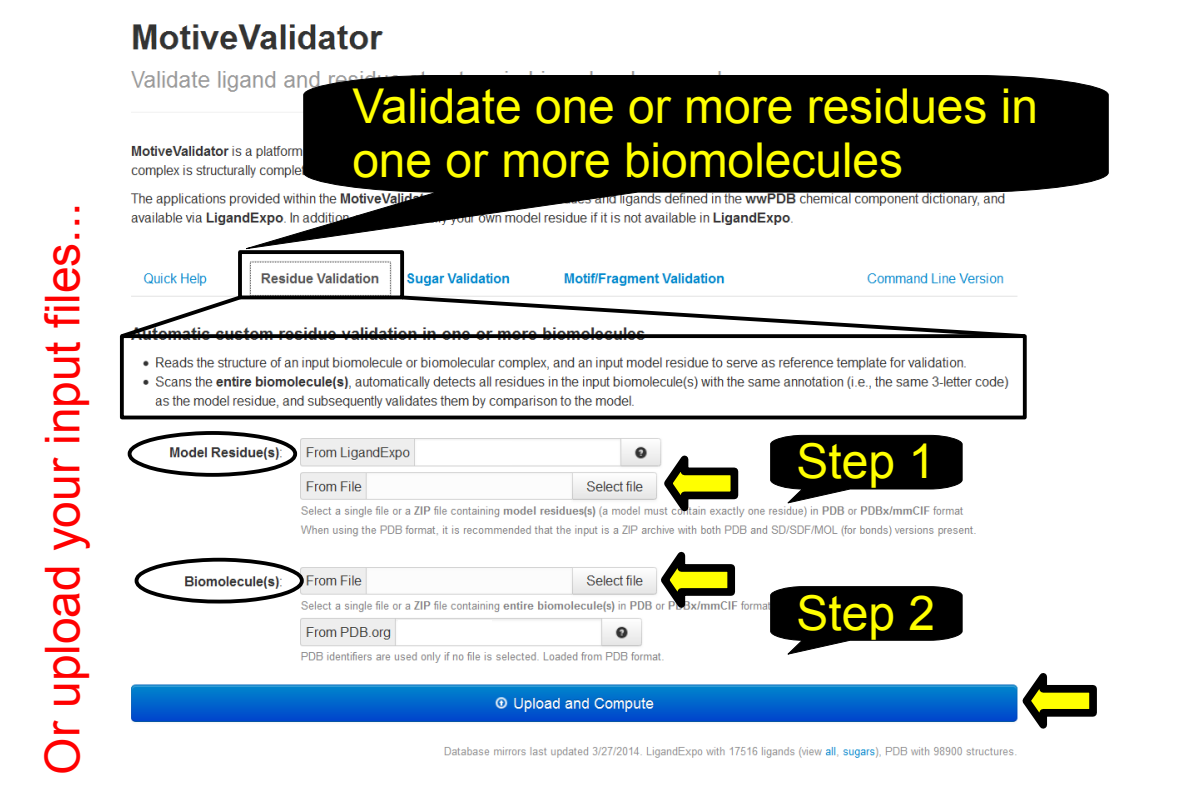

Retrieve input files from databases…
MotiveValidator
Validate ligand and
Validate one or more residues in one or more biomolecules
MotiveValidator is a platform
complex is structurally comple
The applications provided within the MotiveValid
available via LigandExpo. In addition
Quick Help
Residue Validation
Sugar Validation
Motif/Fragment Validation
Command Line Version
Automatic custom residue validation in one or more biomolecules
Reads the structure of an input biomolecule or biomolecular complex, and an input model residue to serve as reference template for validation.
Scans the entire biomolecule(s), automatically detects all residues in the input biomolecule(s) with the same annotation (i.e., the same 3-letter code) as the model residue, and subsequently validates them by comparison to the model.
Model Residue(s):
From LigandExpo
his,arg,trp,glu,
From File
Select file
Select a single file or a ZIP file containing model residues(s) (a model must contain exactly one residue) in PDB or PDBx/mmCIF format
When using the PDB format, it is recommended that the input is a ZIP archive with both PDB and SD/SDF/MOL (for bonds) versions present.
Step 1
Biomolecule(s):
From File
Select file
Select a single file or a ZIP file containing entire biomolecule(s) in PDB or PDBx/mmCIF format
From PDB.org
2dlo,1tqn,2k7w, 4fvu,
PDB identifiers are used only if no file is selected. Loaded from PDB format
Step 2
Upload and Compute
Database mirrors last updated 3/27/2014. LigandExpo with 17516 ligands (view all, sugars), PDB with 98900 structures.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Step 1
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From File
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From PDB.org
PDB identifiers are used only if no file is selected. Loaded from PDB format.
Step 2
Upload and Compute
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Or upload your input files…

MotiveValidator Result

Your results will be available on the server for up to a month

You can come back to the result later using this URL. The result will not be deleted before Saturday, April 19, 2014.

http://webchem.ncbr.muni.cz/Platform/MotiveValidator/Result/LectinsWithMAN

Download Input | Download Result

Summary | Details | Processing Warnings (75)

Method: **Sugar Validation**, computed using version **1.0.14.3.19** on 03/19/2014 15:04:44

- ds the **entire structure** of an input biomolecule or biomolecular complex, automatically detects all sugar (carbohydrate) residues present, subsequently validates them with respect to model residues obtained from the LigandExpo database.
- The structure of each sugar residue in the input structure is compared with the LigandExpo model that has the same annotation, i.e., the same 3-letter residue name according to PDB standards.

A2G AMG BGC BM3 BMA CIS FUC FUL GAL GLA GLC H1M M6P MAN MMA NAG NDG NGZ SIA XYP

Validated residues

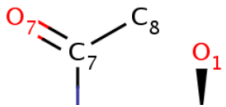
A2G [LigandExpo | PDB | MOL] [$C_8H_{15}N_1O_6$ | n-acetyl-2-deoxy-2-amino-galactose]

5 motifs in 2 structures

Summary

Missing Atoms or Rings			With All Atoms and Rings				
0 (0.00%)			5 (100.00%)				
Rings	Only Atoms	*Different Naming*	Correct Chirality	Wrong Chirality	*Substitutions*	*Foreign*	*Different Naming*
0 (0.00%)	0 (0.00%)	0 (0.00%)	5 (100.00%)	0 (0.00%)	0 (0.00%)	0 (0.00%)	0 (0.00%)

Scroll down to read a summary of the issues found for each residue



MAN [LigandExpo | PDB | MOL] [$C_6H_{12}O_6$ | alpha-d-mannose]
560 motifs in 132 structures, 55 warnings

Validated residue

Summary

Missing Atoms or Rings			With All Atoms and Rings				
8 (1.43%)			552 (98.57%)				
Rings	Only Atoms	*Different Naming*	Correct Chirality	Wrong Chirality	*Substitutions*	*Foreign*	*Different Naming*
0 (0.00%)	8 (1.43%)	0 (0.00%)	522 (93.21%)	30 (5.36%)	0 (0.00%)	361 (64.46%)	0 (0.00%)

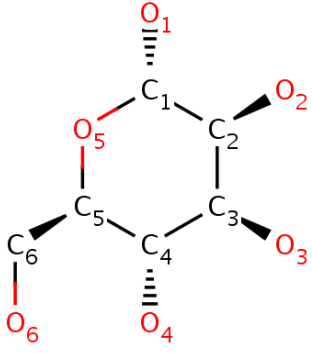
Potential issues identified during validation

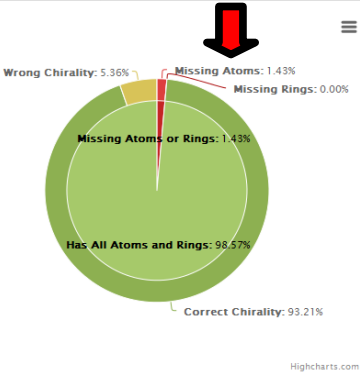
Missing Atoms in 8 motifs with missing atoms but not rings

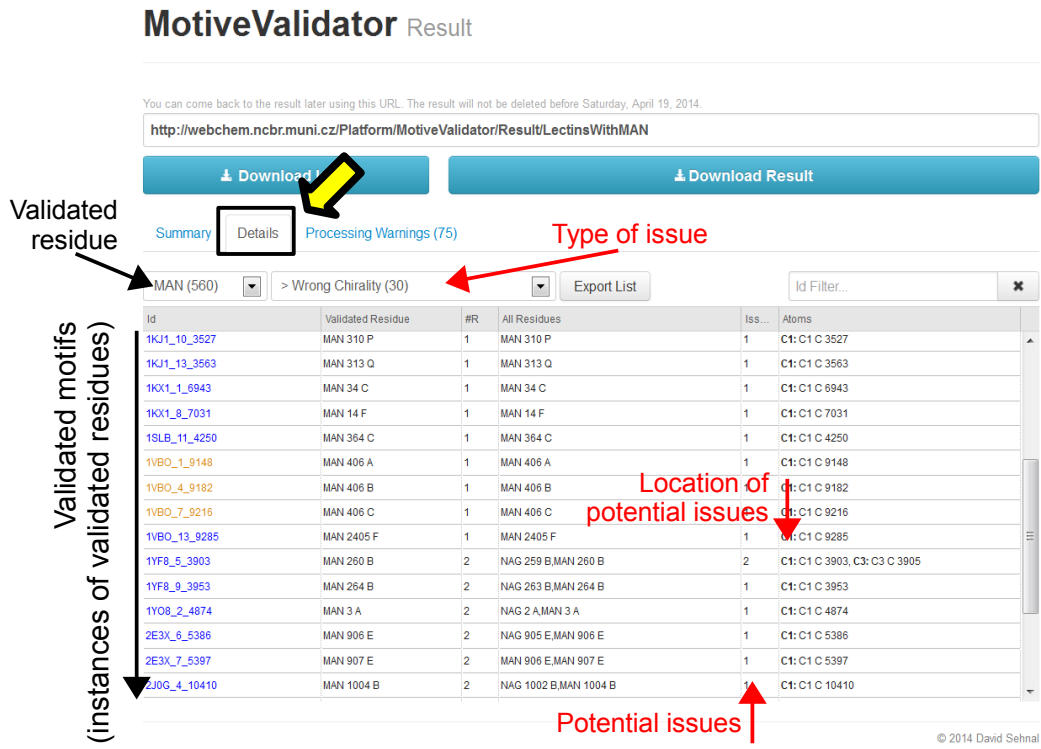
O1	O6
7 (87.50%)	1 (12.50%)

Wrong Chirality in 30 motifs with all atoms

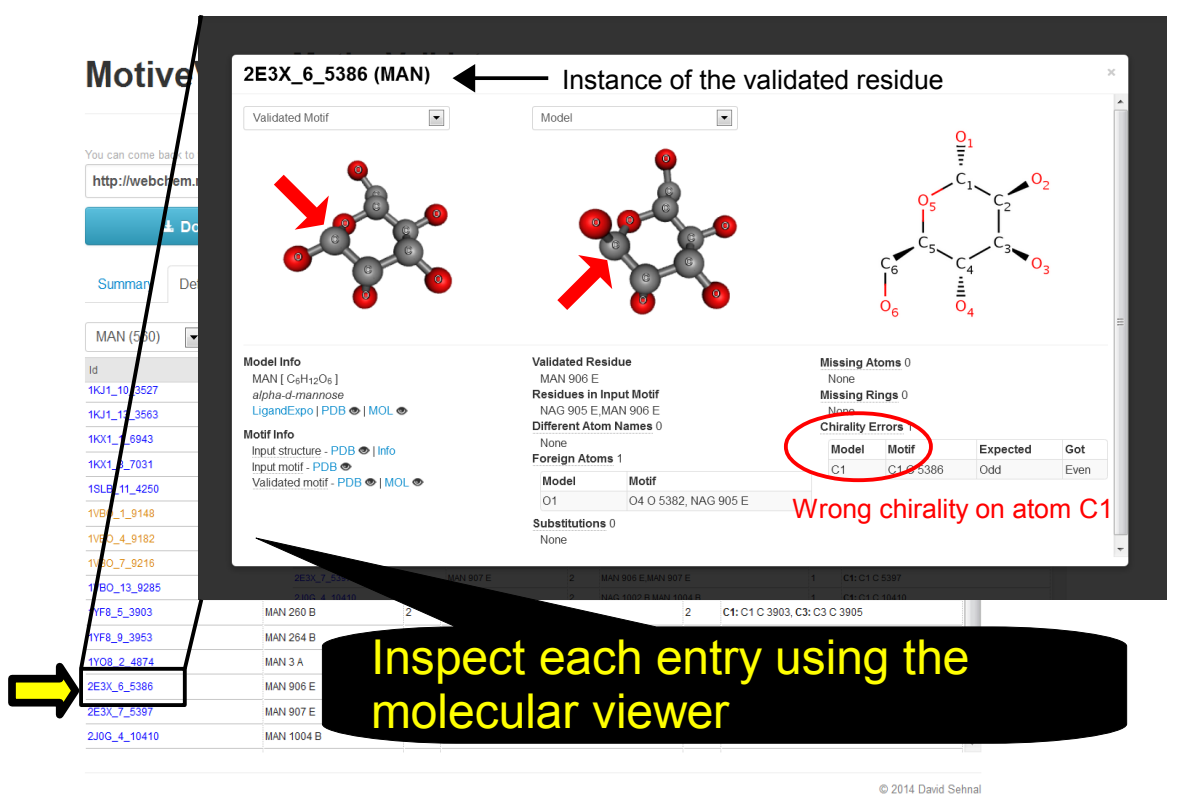
C1	C2	C3
29 (96.67%)	1 (3.33%)	1 (3.33%)
Odd	Even	Even







Id	Validated Residue	#R	All Residues	Iss...	Atoms
1KJ1_10_3527	MAN 310 P	1	MAN 310 P	1	**C1:** C1 C 3527
1KJ1_13_3563	MAN 313 Q	1	MAN 313 Q	1	**C1:** C1 C 3563
1KX1_1_6943	MAN 34 C	1	MAN 34 C	1	**C1:** C1 C 6943
1KX1_8_7031	MAN 14 F	1	MAN 14 F	1	**C1:** C1 C 7031
1SLB_11_4250	MAN 364 C	1	MAN 364 C	1	**C1:** C1 C 4250
1VBO_1_9148	MAN 406 A	1	MAN 406 A	1	**C1:** C1 C 9148
1VBO_4_9182	MAN 406 B	1	MAN 406 B	1	**C1:** C1 C 9182
1VBO_7_9216	MAN 406 C	1	MAN 406 C	1	**C1:** C1 C 9216
1VBO_13_9285	MAN 2405 F	1	MAN 2405 F	1	**C1:** C1 C 9285
1YF8_5_3903	MAN 260 B	2	NAG 259 B,MAN 260 B	2	**C1:** C1 C 3903, **C3:** C3 C 3905
1YF8_9_3953	MAN 264 B	2	NAG 263 B,MAN 264 B	1	**C1:** C1 C 3953
1YO8_2_4874	MAN 3 A	2	NAG 2 A,MAN 3 A	1	**C1:** C1 C 4874
2E3X_6_5386	MAN 906 E	2	NAG 905 E,MAN 906 E	1	**C1:** C1 C 5386
2E3X_7_5397	MAN 907 E	2	MAN 906 E,MAN 907 E	1	**C1:** C1 C 5397
2J0G_4_10410	MAN 1004 B	2	NAG 1002 B,MAN 1004 B	1	**C1:** C1 C 10410


2E3X_6_5386 (MAN)
Instance of the validated residue
Validated Motif
Model
Model Info
MAN [C6H12O6]
alpha-d-mannose
LigandExpo | PDB | MOL
Motif Info
Input structure - PDB | Info
Input motif - PDB
Validated motif - PDB | MOL
Validated Residue
MAN 906 E
Residues in Input Motif
NAG 905 E,MAN 906 E
Different Atom Names 0
None
Foreign Atoms 1
Model
Motif
O1
O4 O 5382, NAG 905 E
Substitutions 0
None
Missing Atoms 0
None
Missing Rings 0
None
Chirality Errors 1
Model
Motif
Expected
Got
C1
C1 C 5386
Odd
Even
Wrong chirality on atom C1
Inspect each entry using the molecular viewer
MAN (5)
Id
1KJ1_10_3527
1KJ1_11_3563
1KX1_1_6943
1KX1_3_7031
1SLB_11_4250
1VBO_1_9148
1VBO_4_9182
1VBO_7_9216
1VBO_13_9285
1YF8_5_3903
1YF8_9_3953
1YO8_2_4874
2E3X_6_5386
2E3X_7_5397
2J0G_4_10410
MAN 260 B
MAN 264 B
MAN 3 A
MAN 906 E
MAN 907 E
MAN 1004 B
C1: C1 C 3903, C3: C3 C 3905
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