PDB entries

**Residues relevant for validation**
(> 6 heavy atoms
no amino acids
no nucleotides)

**VALIDATION**
(complete structure, correct topology and chirality, annotations)

**Residue models**
(reference)

# Validator$^{DB}$

Database of validation results for ligands and residues in the Protein Data Bank.

**Validator$^{DB}$** contains precomputed validation results for ligands and residues in the Protein Data Bank. The database is updated on a weekly basis.

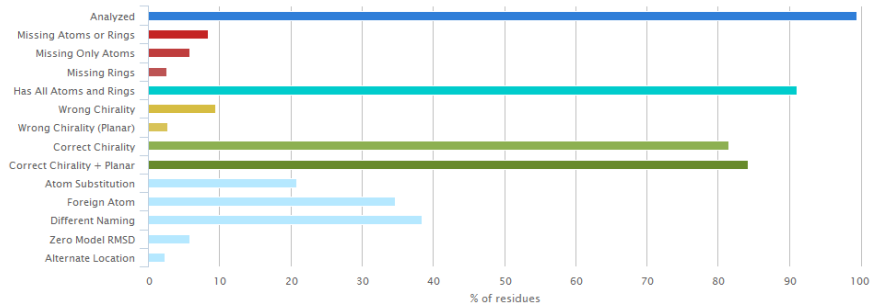
The residues deemed relevant for validation are all ligands and residues with reasonable size (more than six heavy atoms), with the exception of amino acids and nucleotides. The validation is performed using MotiveValidator, and the residue models from wwPDB Chemical Component Dictionary (wwPDB CCD) are used as reference structures for validation.

For a quick tour of the Validator$^{DB}$ features, please view the Tutorial. For a complete description of functionality, along with useful examples, please read the Manual or visit our Wiki pages.

*Database last updated **13/6/2014**: **100843** entries from PDB.org, **232521** residues relevant for validation, **17334** residue models from wwPDB CCD.*

Comma separated list of residue names (3-letter codes) or PDB IDs (4-letter codes). Max 10. Lookup

Overview | Details by Residue | Details by PDB Entry



# ValidatorDB

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General description

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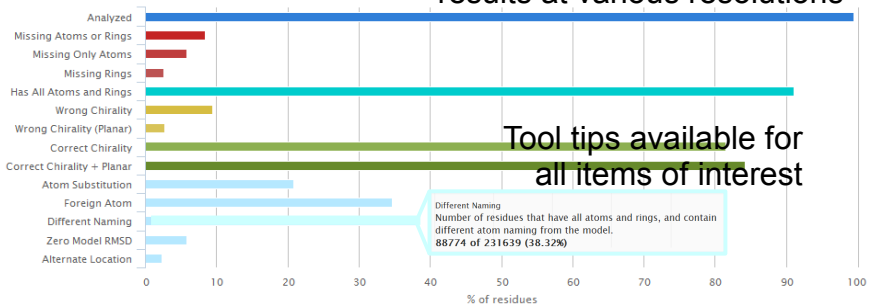
Direct access to detailed validation results for specific residues, or for all relevant residues in specific PDB entries.

*Database last updated **13/6/2014**: **100843** entries from PDB.org, **232521** residues relevant for validation, **17334** residue models from wwPDB CCD.*

Comma separated list of residue names (3-letter codes) or PDB IDs (4-letter codes). Max 10. Lookup

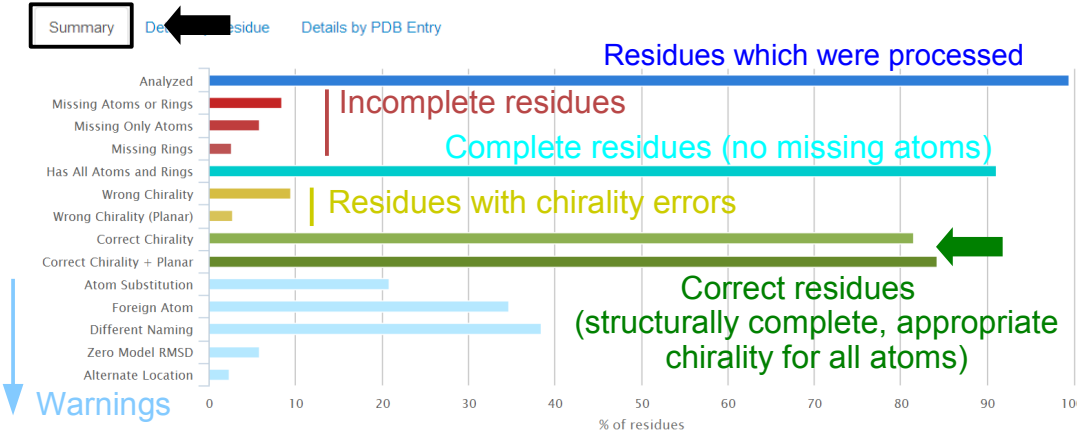
Overview | Details by Residue | Details by PDB Entry

Access to statistics of validation results at various resolutions



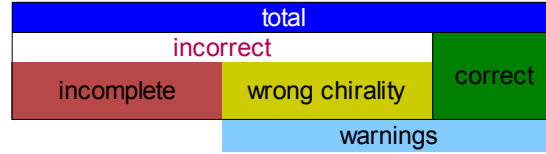

Tool tips available for all items of interest

# Overview of results for the validation of ligands and residues across the entire PDB

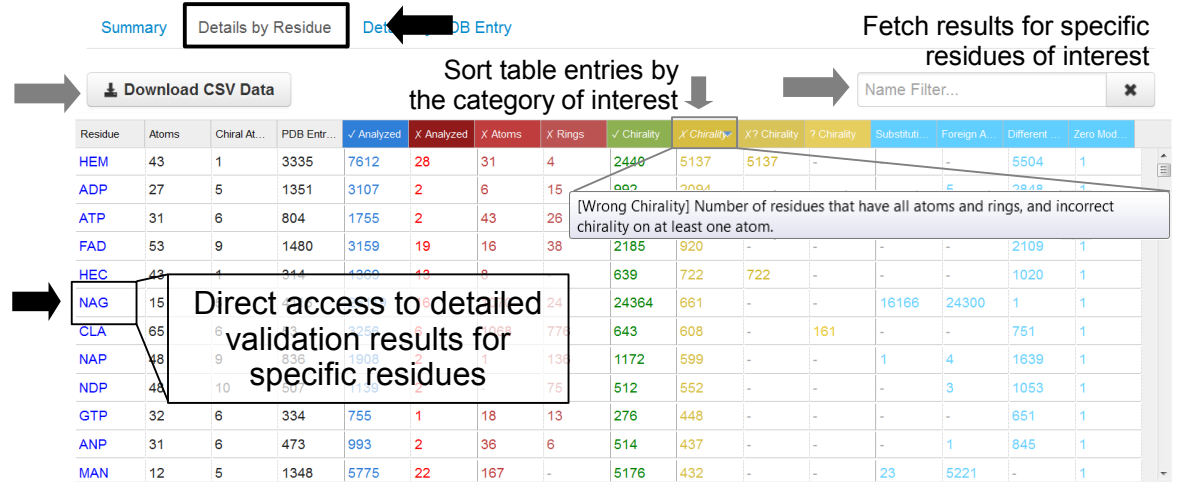



Each analyzed residue is counted as correct if it is complete and has correct chirality on all its atoms. Warnings are given for mild inconsistencies when compared to the model residue serving as reference.

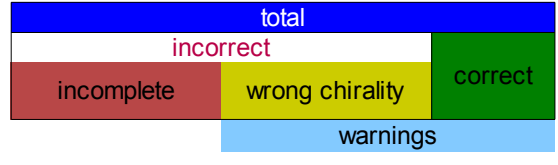
## Color coding



# Overview of validation results for each ligand or residue




Each analyzed residue is counted as correct if it is complete and has correct chirality on all its atoms. Warnings are given for mild inconsistencies when compared to the model residue serving as reference.



# Overview of validation results for each PDB entry

Summary | Details by [illegible] | Details by PDB Entry

Fetch results for specific PDB entries or residues of interest

Download CSV Data

Sort table entries by the category of interest

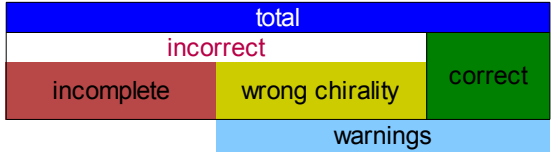
ID or Model Filter...

| PDB ID | Residues | ✓ Analyzed | X Analyzed | X Atoms | X Rings | ✓ Chirality | X Chirality | X? Chirality | ? Chirality | Substituti... | Foreign A... | Different ... | Zero Mod... |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3j00 | PEV PGV | 132 | 1 | - | - | 46 | 86 | - | - | - | - | 56 | - |
| 1rwt | BNG CHL CLA DGD LHG LU... | 210 | - | 40 | - | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] |
| 3a0h | BCR CLA DGD HEM LHG M... | 120 | 4 | - | - | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] | [illegible] |
| 3a0b | BCR CLA DGD HEM LHG M... | 122 | 2 | - | - | 53 | 60 | 1 | 9 | - | - | 54 | - |
| 2j7a | HEM LMT | 90 | - | - | - | 34 | 56 | 56 | - | - | - | 51 | - |
| 2wsc | BCR CLA LMG LMU PQN S... | 256 | - | 119 | 30 | 62 | 56 | - | 7 | - | 1 | 49 | - |
| [illegible] | BCR CLA DGD HEM LHG L... | 172 | 2 | 54 | - | 56 | 56 | 4 | 8 | - | - | 57 | - |
| 2[illegible]e | BCR CLA LMG LMU PQN S... | 251 | - | 104 | 26 | 69 | 53 | - | 5 | 1 | 4 | 45 | - |
| 1h29 | HE[illegible] | 64 | - | - | - | 16 | 48 | 48 | - | - | - | 59 | - |
| 3lw5 | BCR CLA LMG LMU PQN SF4 | 251 | 1 | 103 | 25 | 70 | 46 | - | 7 | - | 1 | 49 | - |
| 2f6a | HYP | 47 | - | 5 | - | - | 42 | - | - | 42 | 42 | 1 | - |
| 2wsf | BCR CLA LMG LMU PQN S... | 256 | - | 119 | 30 | 62 | 40 | - | 5 | - | - | 37 | - |

[Wrong Chirality] Number of residues that have all atoms and rings, and incorrect chirality on at least one atom.

Direct access to detailed validation results for all residues in a specific PDB entry

Each analyzed residue is counted as correct if it is complete and has correct chirality on all its atoms. Warnings are given for mild inconsistencies when compared to the model residue serving as reference.



ValidatorDB

PDB Entry - 1RWT

Detailed validation results for all residues in a specific PDB entry

Summary | Details | Processing Warnings (17) | Overview

BNG CHL CLA DGD LHG LUT NEX XAT

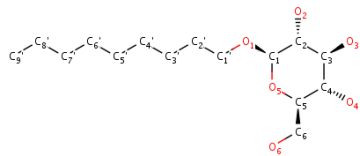
Residues validated in this PDB entry

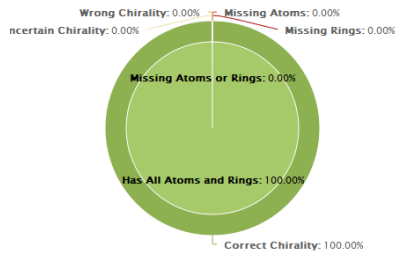
Scroll down for the summary of the issues found for each validated residue

**BNG** [ LigandExpo | PDB | MOL ] [ $C_{15}H_{30}O_6$ | b-nonylglucoside ] [ Chiral Atoms (5): C1, C2, C3, C4, C5 ] [ Experiemental Coordinates ]
10 motifs in 1 structure

**Summary**

| Missing Atoms or Rings | | | With All Atoms and Rings | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 0 (0.00%) | | | 10 (100.00%) | | | | | | |
| Rings | Only Atoms | *Different Naming* | Correct Chirality | Wrong Chirality | *Planar Warn.* | Uncertain Chirality | *Substitutions* | *Foreign* | *Different Naming* |
| 0 (0.00%) | 0 (0.00%) | 0 (0.00%) | 10 (100.00%) | 0 (0.00%) | 0 (0.00%) | 0 (0.00%) | 0 (0.00%) | 0 (0.00%) | 0 (0.00%) |





Validated residue

**CLA** [ LigandExpo | PDB | MOL ] [ $C_{55}H_{72}MgN_4O_5$ | chlorophyll a ] Chiral Atoms (6): MG, C2A, C3A, CBD, C8, C13 ] [ Experiemental Coordinates ]

80 motifs in 1 structure, 7 warnings

Potential issues identified during validation

**Summary**

| Missing Atoms or Rings | | | With All Atoms and Rings | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 20 (25.00%) | | | 60 (75.00%) | | | | | | |
| Rings | Only Atoms | Different Naming | Correct Chirality | Wrong Chirality | Planar Warn. | Uncertain Chirality | Substitutions | Foreign | Different Naming |
| 0 (0.00%) | 20 (25.00%) | 0 (0.00%) | 28 (35.00%) | 25 (31.25%) | 0 (0.00%) | 7 (8.75%) | 0 (0.00%) | 0 (0.00%) | 33 (41.25%) |

**Missing Atoms** in 20 motifs with missing atoms but not rings

| C5 | C6 | C7 | C8 | C9 | C10 | C11 | C12 | C13 | C14 | C15 | C16 | C17 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) | 10 (50.00%) |

| C18 | C19 | C20 |
|---|---|---|
| 20 (100.00%) | 20 (100.00%) | 20 (100.00%) |

Location of missing atom

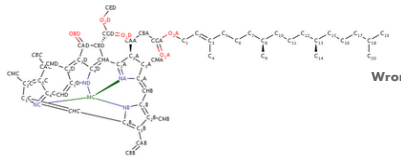
**Wrong Chirality** in 25 motifs with all atoms

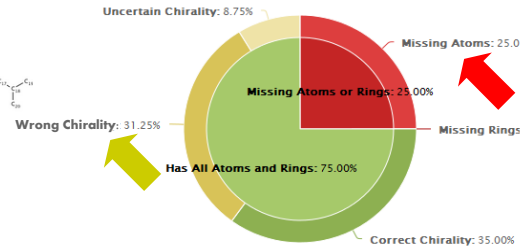
| MG | C8 | C13 |
|---|---|---|
| 13 (52.00%) | 20 (80.00%) | 2 (8.00%) |

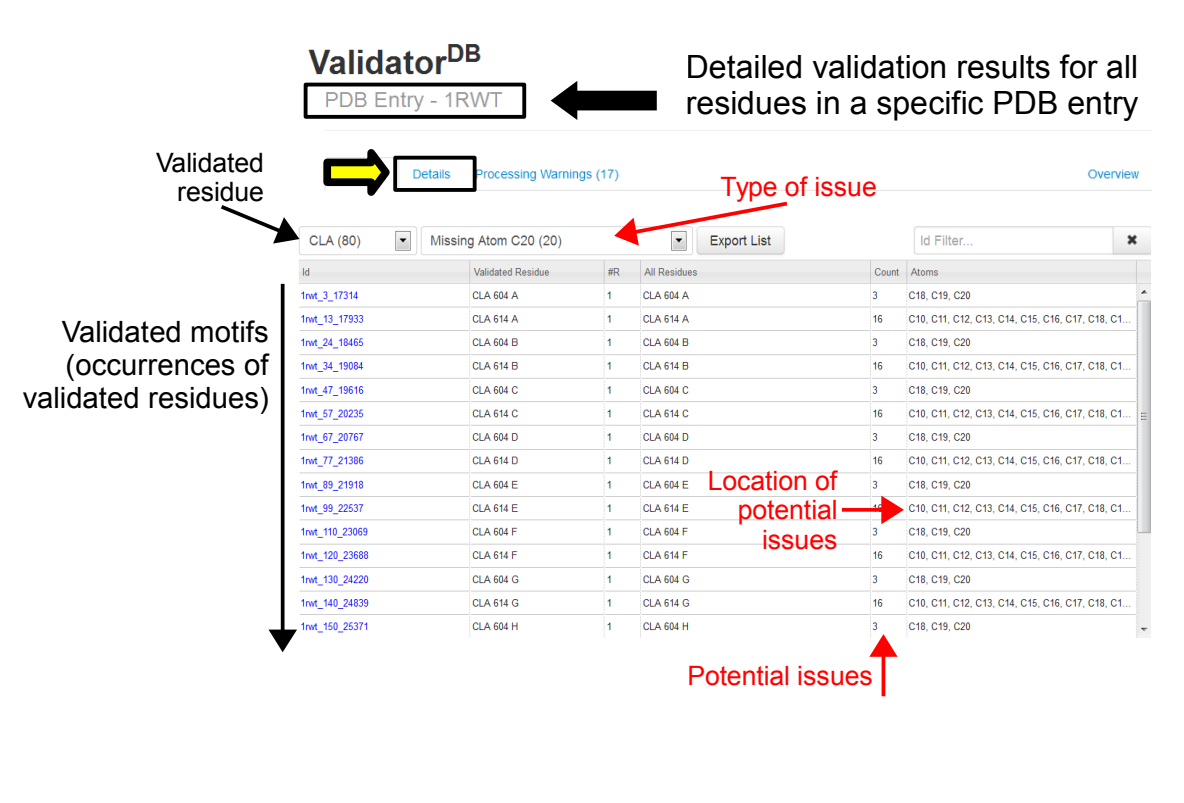
Location of wrong chirality

Download figure

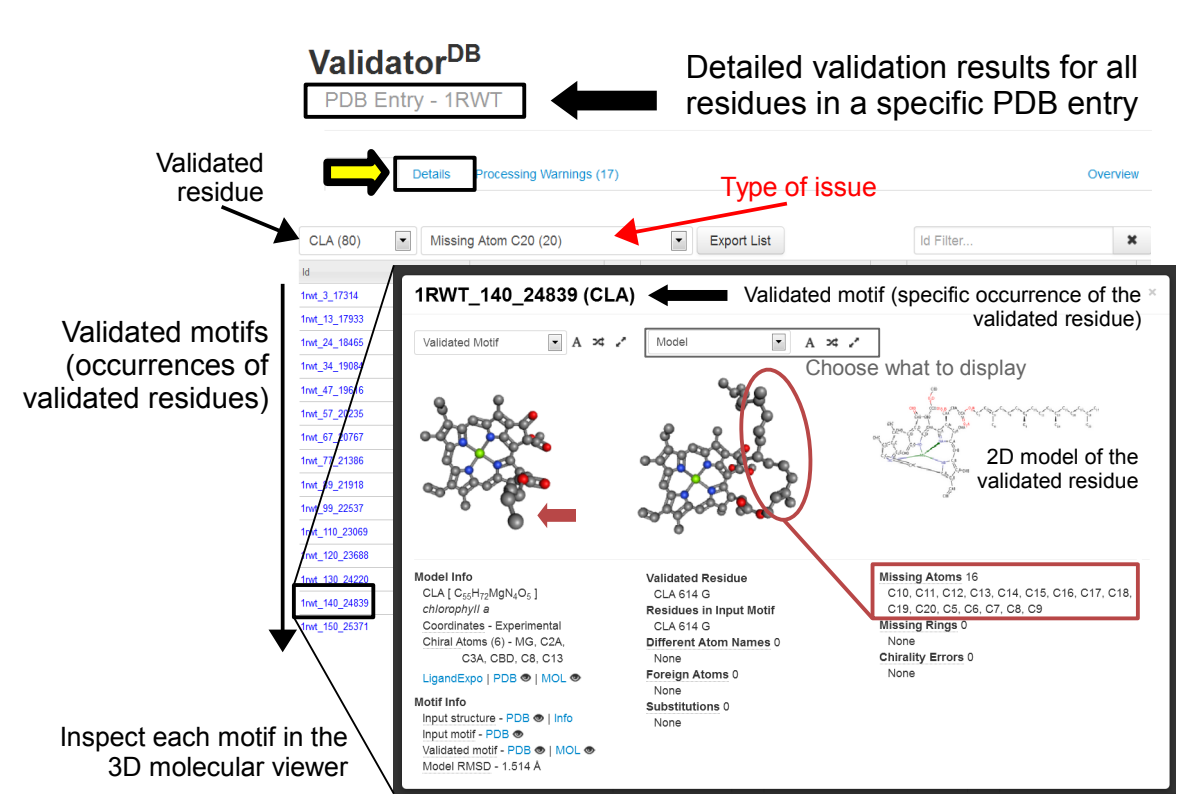
2D model of the validated residue








| Id | Validated Residue | #R | All Residues | Count | Atoms |
|---|---|---|---|---|---|
| 1rwt_3_17314 | CLA 604 A | 1 | CLA 604 A | 3 | C18, C19, C20 |
| 1rwt_13_17933 | CLA 614 A | 1 | CLA 614 A | 16 | C10, C11, C12, C13, C14, C15, C16, C17, C18, C1... |
| 1rwt_24_18465 | CLA 604 B | 1 | CLA 604 B | 3 | C18, C19, C20 |
| 1rwt_34_19084 | CLA 614 B | 1 | CLA 614 B | 16 | C10, C11, C12, C13, C14, C15, C16, C17, C18, C1... |
| 1rwt_47_19616 | CLA 604 C | 1 | CLA 604 C | 3 | C18, C19, C20 |
| 1rwt_57_20235 | CLA 614 C | 1 | CLA 614 C | 16 | C10, C11, C12, C13, C14, C15, C16, C17, C18, C1... |
| 1rwt_67_20767 | CLA 604 D | 1 | CLA 604 D | 3 | C18, C19, C20 |
| 1rwt_77_21386 | CLA 614 D | 1 | CLA 614 D | 16 | C10, C11, C12, C13, C14, C15, C16, C17, C18, C1... |
| 1rwt_89_21918 | CLA 604 E | 1 | CLA 604 E | 3 | C18, C19, C20 |
| 1rwt_99_22537 | CLA 614 E | 1 | CLA 614 E | 16 | C10, C11, C12, C13, C14, C15, C16, C17, C18, C1... |
| 1rwt_110_23069 | CLA 604 F | 1 | CLA 604 F | 3 | C18, C19, C20 |
| 1rwt_120_23688 | CLA 614 F | 1 | CLA 614 F | 16 | C10, C11, C12, C13, C14, C15, C16, C17, C18, C1... |
| 1rwt_130_24220 | CLA 604 G | 1 | CLA 604 G | 3 | C18, C19, C20 |
| 1rwt_140_24839 | CLA 614 G | 1 | CLA 614 G | 16 | C10, C11, C12, C13, C14, C15, C16, C17, C18, C1... |
| 1rwt_150_25371 | CLA 604 H | 1 | CLA 604 H | 3 | C18, C19, C20 |


ValidatorDB
PDB Entry - 1RWT
Detailed validation results for all residues in a specific PDB entry
Validated residue
Details
Processing Warnings (17)
Overview
Type of issue
CLA (80)
Missing Atom C20 (20)
Export List
Id Filter...
Id
1rwt_3_17314
1rwt_13_17933
1rwt_24_18465
1rwt_34_19086
1rwt_47_19616
1rwt_57_20235
1rwt_67_20767
1rwt_77_21386
1rwt_89_21918
1rwt_99_22537
1rwt_110_23069
1rwt_120_23688
1rwt_130_24220
1rwt_140_24839
1rwt_150_25371
Validated motifs (occurrences of validated residues)
1RWT_140_24839 (CLA)
Validated motif (specific occurrence of the validated residue)
Validated Motif
Model
Choose what to display
2D model of the validated residue
Model Info
CLA [ C55H72MgN4O5 ]
chlorophyll a
Coordinates - Experimental
Chiral Atoms (6) - MG, C2A, C3A, CBD, C8, C13
LigandExpo | PDB | MOL
Motif Info
Input structure - PDB | Info
Input motif - PDB
Validated motif - PDB | MOL
Model RMSD - 1.514 Å
Validated Residue
CLA 614 G
Residues in Input Motif
CLA 614 G
Different Atom Names 0
None
Foreign Atoms 0
None
Substitutions 0
None
Missing Atoms 16
C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C5, C6, C7, C8, C9
Missing Rings 0
None
Chirality Errors 0
None
Inspect each motif in the 3D molecular viewer

ValidatorDB

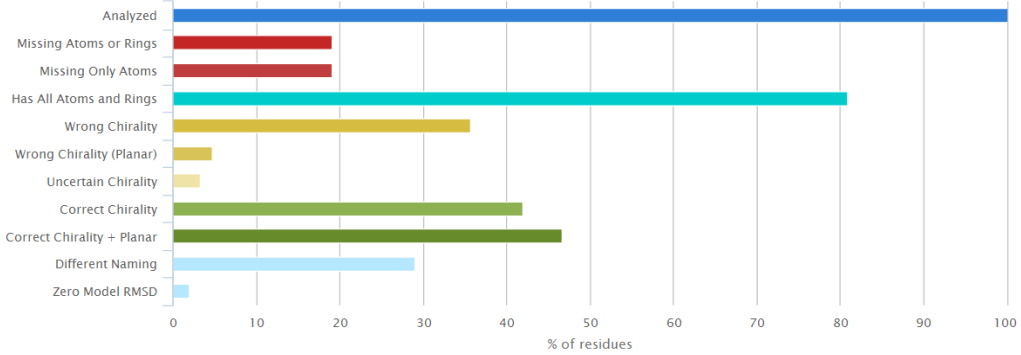
PDB Entry - 1RWT

Detailed validation results for all residues in a specific PDB entry

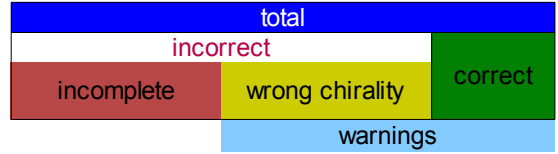
Summary | Details | Processing Warnings (17) | Overview

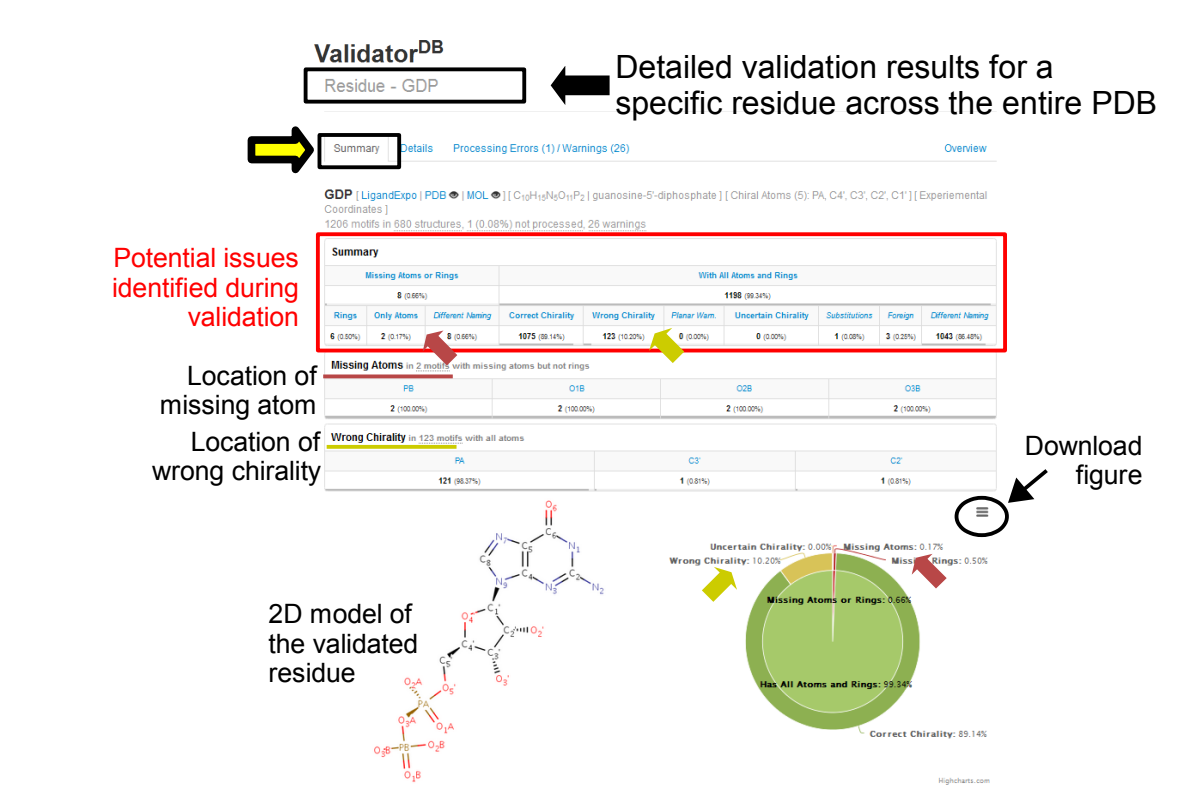
*Validated 210 motifs in 1 structure.*

Motifs = specific occurrences of validated residues




Each analyzed residue is counted as correct if it is complete and has correct chirality on all its atoms. Warnings are given for mild inconsistencies when compared to the model residue serving as reference.




ValidatorDB
Residue - GDP
Detailed validation results for a specific residue across the entire PDB
Summary
Details
Processing Errors (1) / Warnings (26)
Overview
GDP [ LigandExpo | PDB | MOL ] [ C10H15N5O11P2 | guanosine-5'-diphosphate ] [ Chiral Atoms (5): PA, C4', C3', C2', C1' ] [ Experimental Coordinates ]
1206 motifs in 680 structures, 1 (0.08%) not processed, 26 warnings
Potential issues identified during validation
Summary
Missing Atoms or Rings
With All Atoms and Rings
8 (0.66%)
1198 (99.34%)
Rings
Only Atoms
Different Naming
Correct Chirality
Wrong Chirality
Planar Warn.
Uncertain Chirality
Substitutions
Foreign
Different Naming
6 (0.50%)
2 (0.17%)
8 (0.66%)
1075 (89.14%)
123 (10.20%)
0 (0.00%)
0 (0.00%)
1 (0.08%)
3 (0.25%)
1043 (86.48%)
Location of missing atom
Missing Atoms in 2 motifs with missing atoms but not rings
PB
O1B
O2B
O3B
2 (100.00%)
2 (100.00%)
2 (100.00%)
2 (100.00%)
Location of wrong chirality
Wrong Chirality in 123 motifs with all atoms
PA
C3'
C2'
121 (98.37%)
1 (0.81%)
1 (0.81%)
Download figure
2D model of the validated residue
Uncertain Chirality: 0.00%
Missing Atoms: 0.17%
Wrong Chirality: 10.20%
Missing Rings: 0.50%
Missing Atoms or Rings: 0.66%
Has All Atoms and Rings: 99.34%
Correct Chirality: 89.14%
Highcharts.com