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)

MotiveValidator^{DB}

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

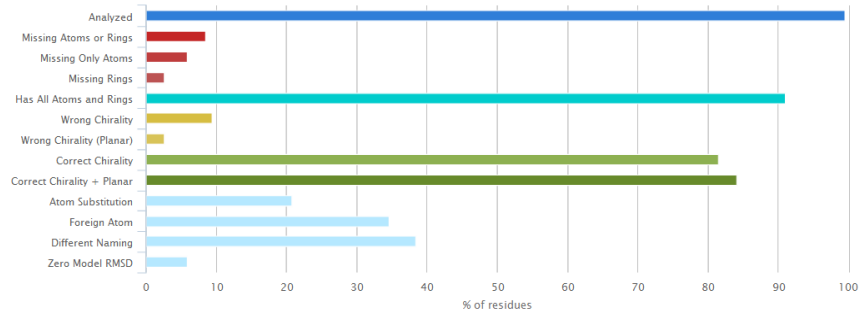
MotiveValidator^{DB} contains precomputed validation results for ligands and residues in the Protein Data Bank. The database is updated on a weekly basis.

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.

*Database last updated **30/5/2014**: **100547** entries from PDB.org, **231639** residues relevant for validation, **17320** residue models from wwPDB CCD.*

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

Summary | Details by Residue | Details by PDB Entry



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MotiveValidator^{DB}

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

General description

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

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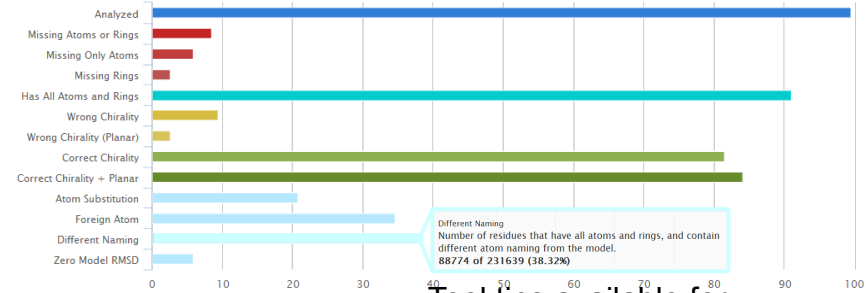
*Database last updated **30/5/2014**: **100547** entries from PDB.org, **231639** residues relevant for validation, **17320** residue models from wwPDB CCD.*

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

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

Summary | Details by Residue | Details by PDB Entry

Access to statistics of validation results at various resolutions



Tool tips available for all items of interest

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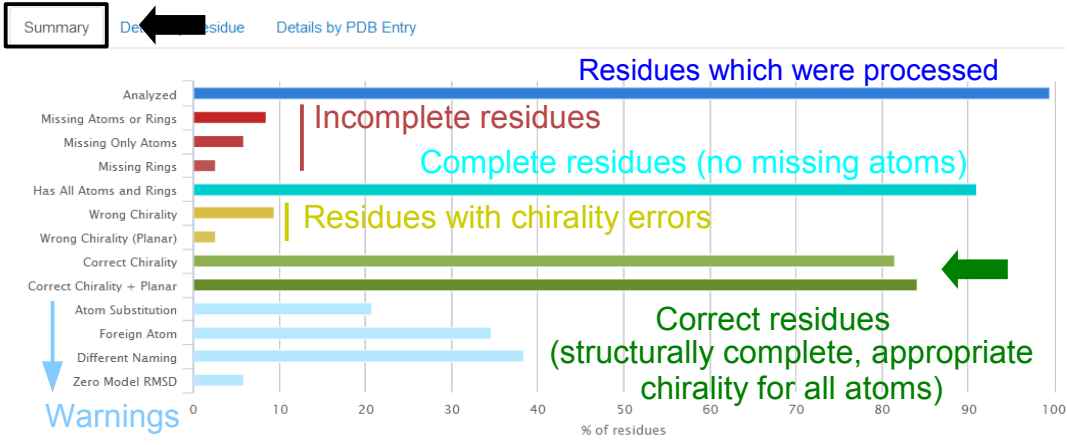
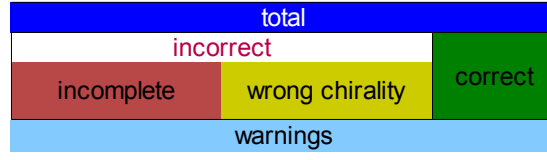
Overview of results for the validation of ligands and residues across the entire PDB

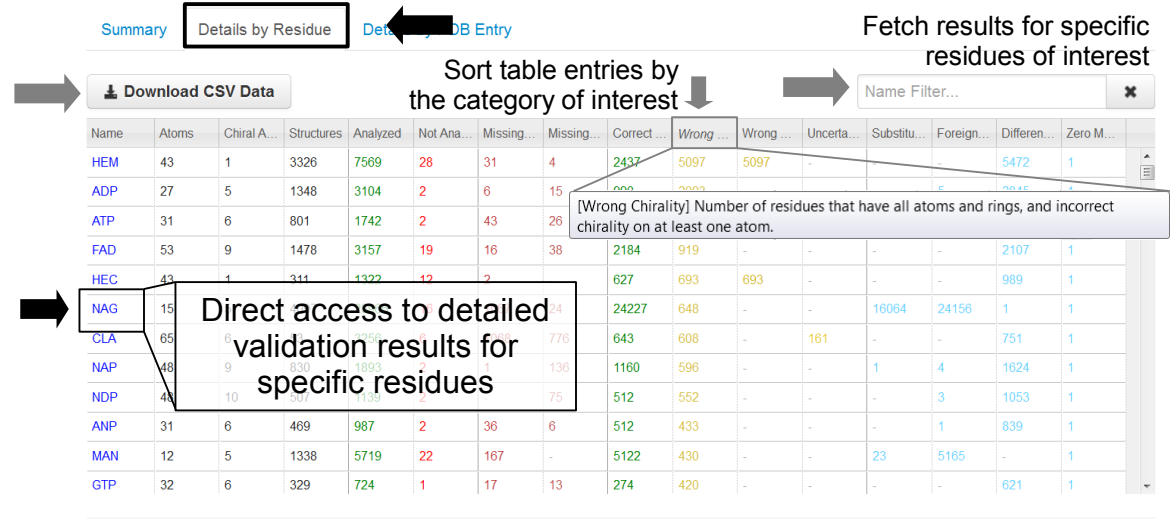


Each analyzed residue is counted as correct if it is complete and has correct chirality on all its atoms. Warnings are given for mild inconsistencies when compared to the model residue serving as reference.

Color coding

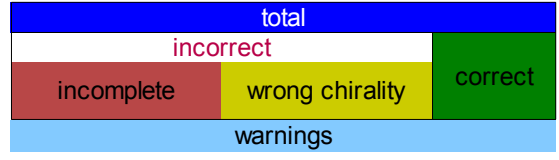


Overview of validation results for each ligand or residue

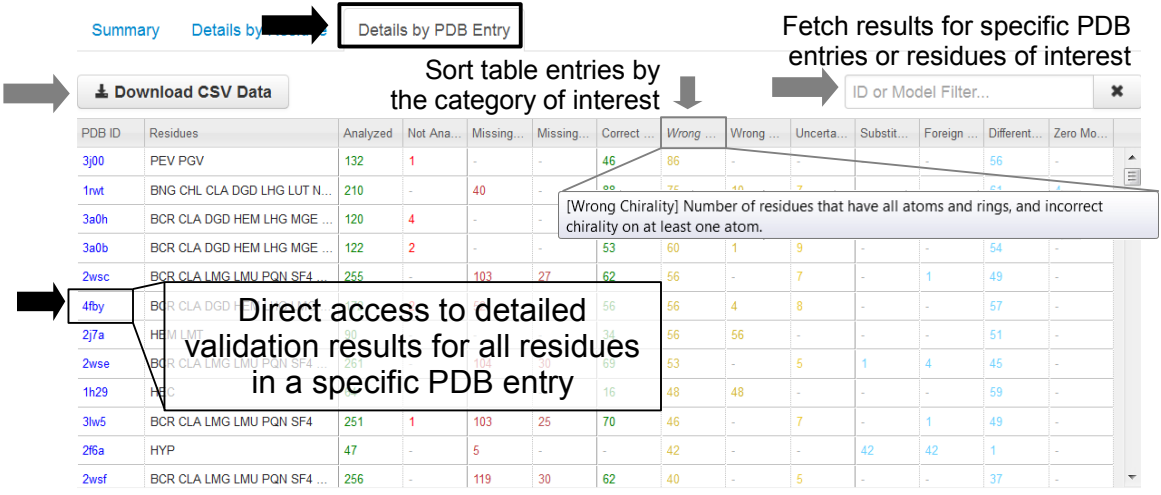


Name	Atoms	Chiral A...	Structures	Analyzed	Not Ana...	Missing...	Missing...	Correct ...	*Wrong ...*	Wrong ...	Uncerta...	Substitu...	Foreign...	Differen...	Zero M...
HEM	43	1	3326	7569	28	31	4	2437	5097	5097				5472	1
ADP	27	5	1348	3104	2	6	15								
ATP	31	6	801	1742	2	43	26								
FAD	53	9	1478	3157	19	16	38	2184	919	-	-	-	-	2107	1
HEC	43	1	311	1322	12	2		627	693	693	-	-	-	989	1
NAG	15							24227	648	-	-	16064	24156	1	1
CLA	65	6					776	643	608	-	161	-	-	751	1
NAP	48	9	830	1893	1	1	136	1160	596	-	-	1	4	1624	1
NDP	48	10	507	1139	2	1	75	512	552	-	-	-	3	1053	1
ANP	31	6	469	987	2	36	6	512	433	-	-	-	1	839	1
MAN	12	5	1338	5719	22	167	-	5122	430	-	-	23	5165	-	1
GTP	32	6	329	724	1	17	13	274	420	-	-	-	-	621	1

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.

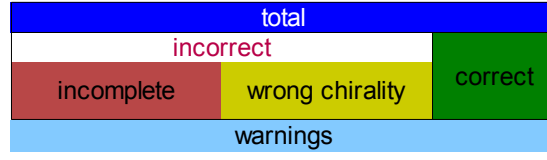


Overview of validation results for each PDB entry



PDB ID	Residues	Analyzed	Not Ana...	Missing...	Missing...	Correct ...	*Wrong ...*	Wrong ...	Uncerta...	Substit...	Foreign ...	Different...	Zero Mo...
3j00	PEV PGV	132	1	-	-	46	86	-	-		-	56	-
1rwt	BNG CHL CLA DGD LHG LUT N...	210	-	40	-	88	75	10	7			61	4
3a0h	BCR CLA DGD HEM LHG MGE ...	120	4	-	-								
3a0b	BCR CLA DGD HEM LHG MGE ...	122	2	-	-	53	60	1	9	-	-	54	-
2wsc	BCR CLA LMG LMU PQN SF4 ...	255	-	103	27	62	56	-	7	-	1	49	-
4fby	BCR CLA DGD H...					56	56	4	8	-	-	57	-
2j7a	HEM LMT	90				34	56	56	-	-	-	51	-
2wse	BCR CLA LMG LMU PQN SF4 ...	261				69	53	-	5	1	4	45	-
1h29	HEC					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 SF4 ...	256	-	119	30	62	40	-	5	-	-	37	-

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.



MotiveValidator^{DB}

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

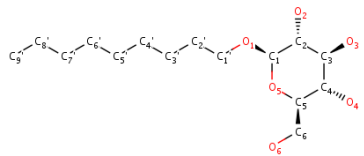
Residues validated in this PDB entry

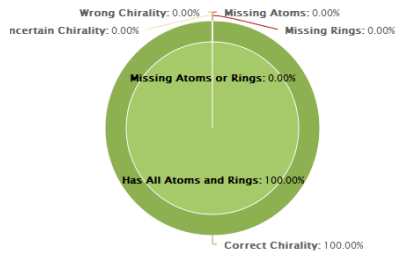
Scroll down for the summary of the issues found for each validated residue

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

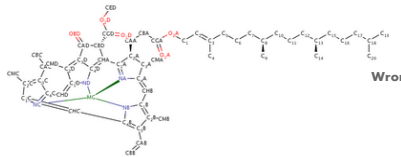
Wrong Chirality in 25 motifs with all atoms

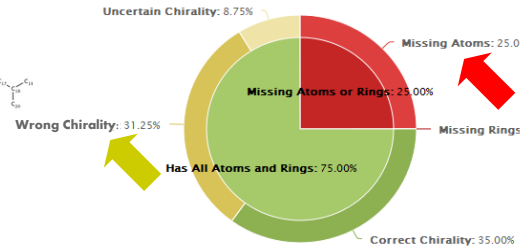
MG	C8	C13
13 (52.00%)	20 (80.00%)	2 (8.00%)

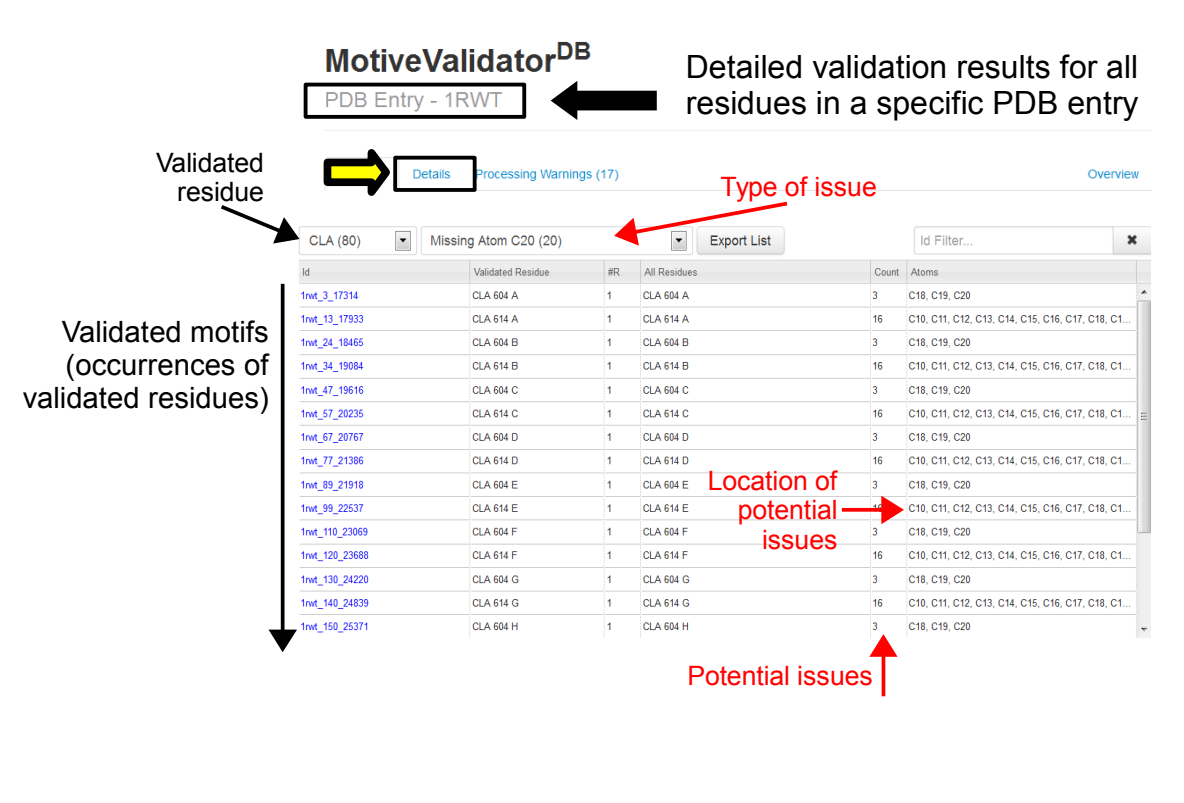
Location of wrong chirality

Download figure

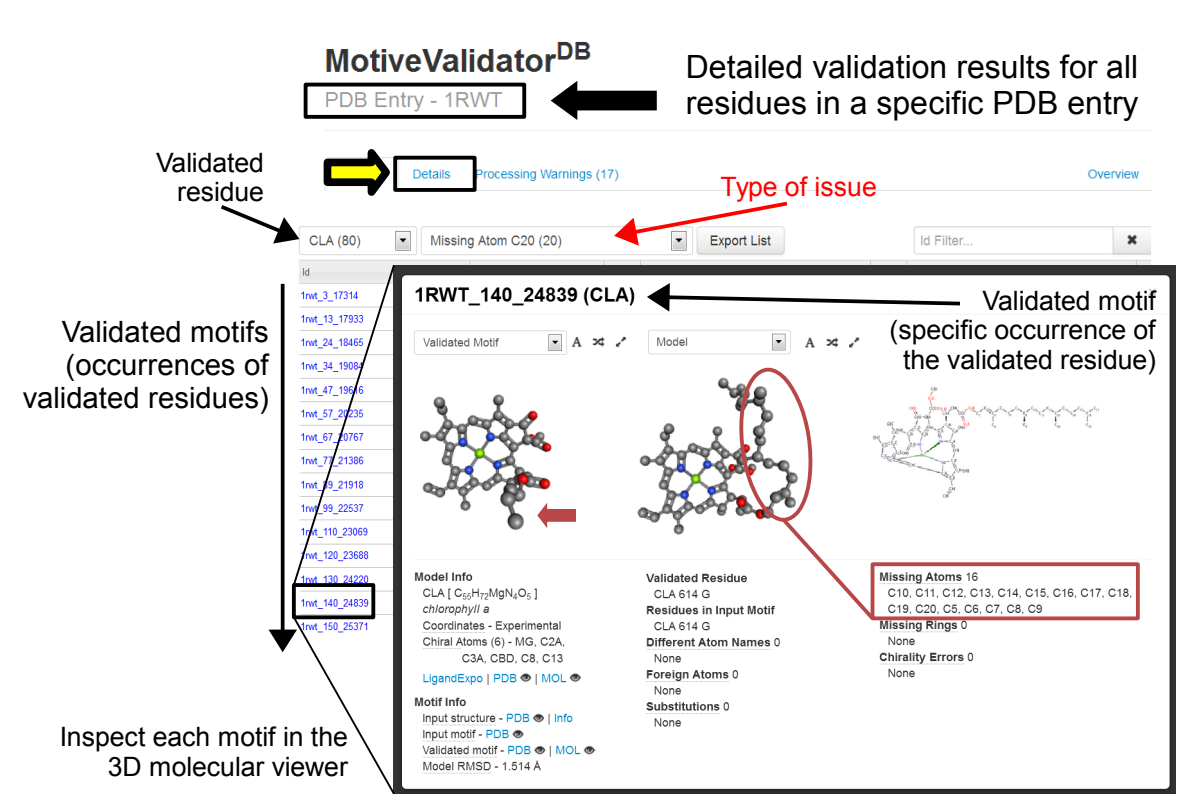
2D model of the validated residue







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


MotiveValidator DB
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_19084
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
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

MotiveValidator^{DB}

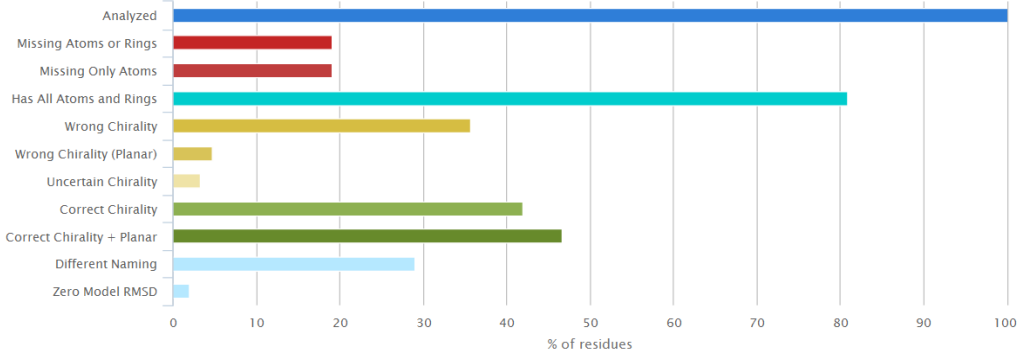
PDB Entry - 1RWT

Detailed validation results for all residues in a specific PDB entry

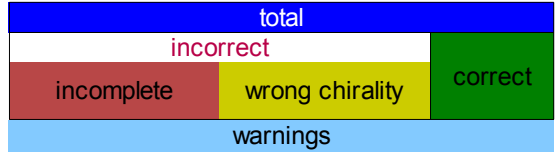
Summary | Details | Processing Warnings (17) | Overview

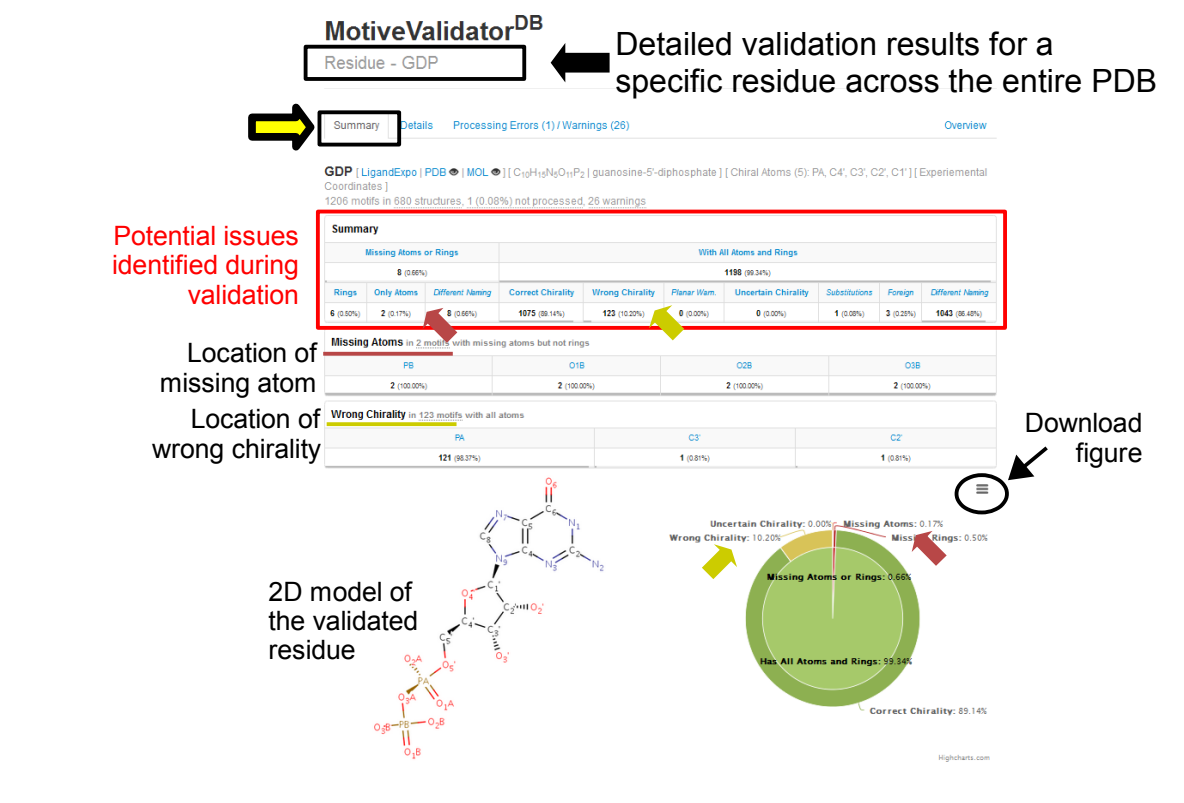
Validated 210 motifs in 1 structure.

Motifs = specific occurrences of validated residues



Each analyzed motif 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.




MotiveValidator DB
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'] [Experiemental 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 Wrm.
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