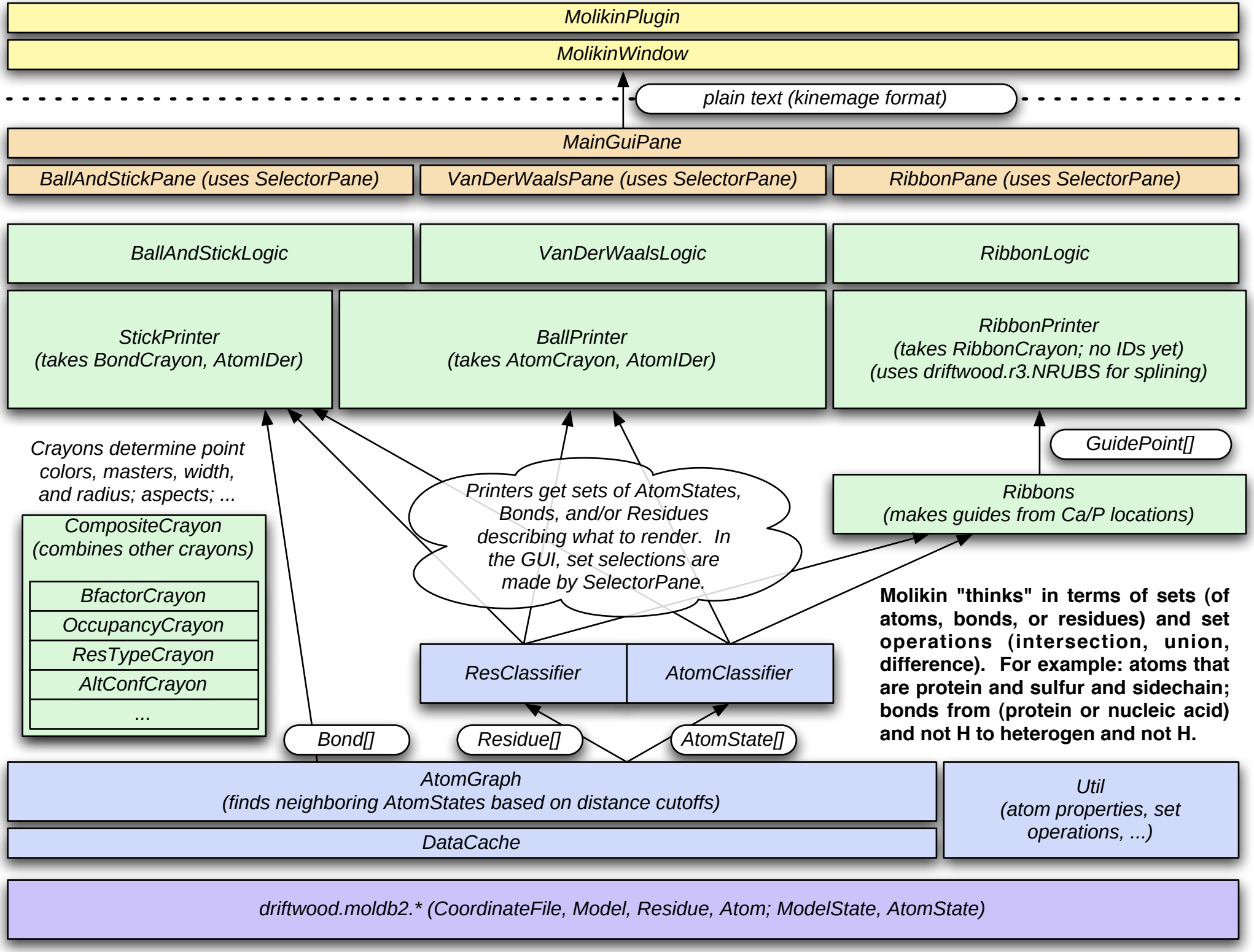
MolikinPlugin
MolikinWindow
plain text (kinemage format)
MainGuiPane
BallAndStickPane (uses SelectorPane)
VanDerWaalsPane (uses SelectorPane)
RibbonPane (uses SelectorPane)
BallAndStickLogic
VanDerWaalsLogic
RibbonLogic
StickPrinter
(takes BondCrayon, AtomIDer)
BallPrinter
(takes AtomCrayon, AtomIDer)
RibbonPrinter
(takes RibbonCrayon; no IDs yet)
(uses driftwood.r3.NRUBS for splining)
GuidePoint[]
Ribbons
(makes guides from Ca/P locations)
Crayons determine point colors, masters, width, and radius; aspects; ...
CompositeCrayon
(combines other crayons)
BfactorCrayon
OccupancyCrayon
ResTypeCrayon
AltConfCrayon
...
Printers get sets of AtomStates, Bonds, and/or Residues describing what to render. In the GUI, set selections are made by SelectorPane.
ResClassifier
AtomClassifier
Molikin "thinks" in terms of sets (of atoms, bonds, or residues) and set operations (intersection, union, difference). For example: atoms that are protein and sulfur and sidechain; bonds from (protein or nucleic acid) and not H to heterogen and not H.
Bond[]
Residue[]
AtomState[]
AtomGraph
(finds neighboring AtomStates based on distance cutoffs)
DataCache
Util
(atom properties, set operations, ...)
driftwood.moldb2.* (CoordinateFile, Model, Residue, Atom; ModelState, AtomState)