CHANGELOG

Notable changes are listed

Version 1.1 - September 26, 2012

- Extend chain... option now available

Version 1.0.2 - August 9, 2012

- Bug fix: RCrane now preserves segids when rotamerizing. This bug was causing issues when structures were rotamerized with RCrane and then refined with Phenix. (reported by Nat Echols)

Version 1.0.1 - May 4, 2012 (internal release)

- Minor update to ensure compatability with future releases of Coot

Version 1.0 - April 16, 2012

- RCrane is now distributed with Coot (accessed via Extensions -> RCrane launch). RCrane 1.0 is included with Coot 0.7.
- The first time RCrane is run, a pop-up now appears informing the user of the appropriate citation for RCrane. This pop-up contains a Don't show again checkbox that will prevent it from re-appearing.
- A number of behind the scenes changes to make RCrane easier to distribute with Coot

Version 0.10 - April 3, 2012

- Rotamerize without density... option now available. This option performs a rotamerization, but completely ignored the electron density. This is primarily intended to be used when building theoretical models (i.e. building without any electron density present).
- RCrane molecules are now named "RCrane-molecule-#" instead of "RCrane molecule #" (i.e. dashes in place of spaces). Now, when the molecules are saved, the filename will not have spaces, as filenames with spaces can cause problems for a few other crystallography programs. (Requested by Maco Marcia)
- RCrane can now optionally use the new Phenix/MolProbity pucker-specific restraint parameters. Enabled with rcrane.enablePhenixRestraints() (Requested by Sri Somarowthu)
- Nucleotides created using RCrane now follow the standard atom ordering when saved as a PDB file (requested by Hasan Demirci)

- Bug fix: During backbone tracing, mutating or flipping a base while a Manually Adjust window is open no longer causes incorrect behavior.
- Bug fix: A progress bar is now displayed when calculating coordinates for a single nucleotide.
- Bug fix: when rotamerizing, selecting alternate conformers for the first (or last) nucleotide will properly retain the torsions for the preceeding (or following) heminucleotide.
- Bug fix: When rotamerizing, changing the starting pucker of the first nucleotide no longer results in an error message.

Version 0.9 - October 26, 2011

- Rotamerization now functions properly when hydrogen atoms are present. RCrane will now remove all hydrogen atoms from rotamerized nucleotides. Previously, hydrogen atoms were allowed to float freely during minimization.
- RCrane now displays an appropriate error message if the user attempts to rotamerize a modified nucleotide. Previously, RCrane would fail with an error about a missing N1/9 atom. Future support for rotamerizing modified nucleotides is planned.
- RCrane now limits the number of nucleotides that can be rotamerized at once. The default limit is 20. This is done to prevent excessivly long run times due to an erroneous mouse click. To increase the limit, use the Python command rcrane.setRotamerizeMaxNucleotides(40). To remove the limit, use the Python command rcrane.setRotamerizeMaxNucleotides(-1).

Version 0.8 - August 26, 2011

- Bug fix: Rotamerization occasionally added a dummy atom to the end of the chain (reported by Francis Reyes)
- RCrane now displays an error if the user attempts to rotamerize a structure with anisotropic temperature factors when using versions of Coot older than 0.7-pre r3631. Previously, attempts to rotamerize structures with aniostropic temperature factors would fail without an obvious error message. (reported by Francis Reyes)

Version 0.7 - August 10, 2011

- Can now trace structures 3'->5' in addition to 5'->3' (suggested by Gregor Blaha)
- Keyboard shortcut for a 5'->3' trace is now controlled by the rcrane_keyboard_shortcut_trace3 variable rather than rcrane_keyboard_shortcut

- Keyboard shortcut for a 3'->5' trace can now be set using the rcrane_keyboard_shortcut_trace5 (defaults to Shift+M). The keyboard shortcut for rotamerization can be set using rcrane_keyboard_shortcut_rotamerize (defaults to no shortcut)
- RCrane no longer minimizes terminal 3' oxygens for alternate conformers or rotamerizations. This speeds up minimization and avoids certain minimization errors.
- Bug fix: now works with negative residue numbers
- Requires Coot 0.6.2 or newer

Version 0.6 - July 11, 2011

- Now using PDB3 naming instead of PDB2 due to the new Coot monomer library
- Improved minimization of high-anti nucleotides
- Bug fix: Installation under Windows would fail for certain paths
- Bug fix: Building a single nucleotide now works (Note that no conformer prediction can occur with only a single nucleotide.)
- Requires Coot r3489 (0.6.2-pre) or greater

Version 0.5 - June 16, 2011

- The interface for reviewing suites now includes an overview listing all built suites (suggested by Gregor Blaha)
- The README now includes instructions for installing RCrane for all users of a computer
- Bug fix: The C3' atom of the previous residue was sometimes slightly moved when selecting an alternate conformer

Version 0.4 - June 7, 2011

- Wannabe rotamers added (2g, 2u, 2z, 3g, 5n, 5r)
- Phosphate search results are now cached between traces, which dramatically speeds up subsequent new traces (requested by Gregor Blaha)
- Added ability to rotamerize existing regions of structure. This uses already-built phosphate and base coordinates to predict new conformers and rebuilt the backbone.

Version 0.3 - March 30, 2011 (initial public release)

- Coordinate calculation now uses start position (harmonic) restraints for base and phosphate atoms of the current nucleotide
- Improved minimization of syn nucleotides

- Added install script
- RCrane now manually draws backbone bonds that are too long for Coot to draw
- Backbone tracing will automatically begin after selecting a refinement map when starting RCrane with no map selected (suggested by Francis Reyes)
- Mouse wheel now moves adjustment sliders by a usable amount (suggested by Francis Reyes)
- Requires Coot r3440 (0.6.2-pre) or greater

Version 0.2 - February 1, 2011 (closed beta)

- Requires Coot r3256 (0.6.2-pre) or greater

Version 0.1 - November, 2010 (internal release)