



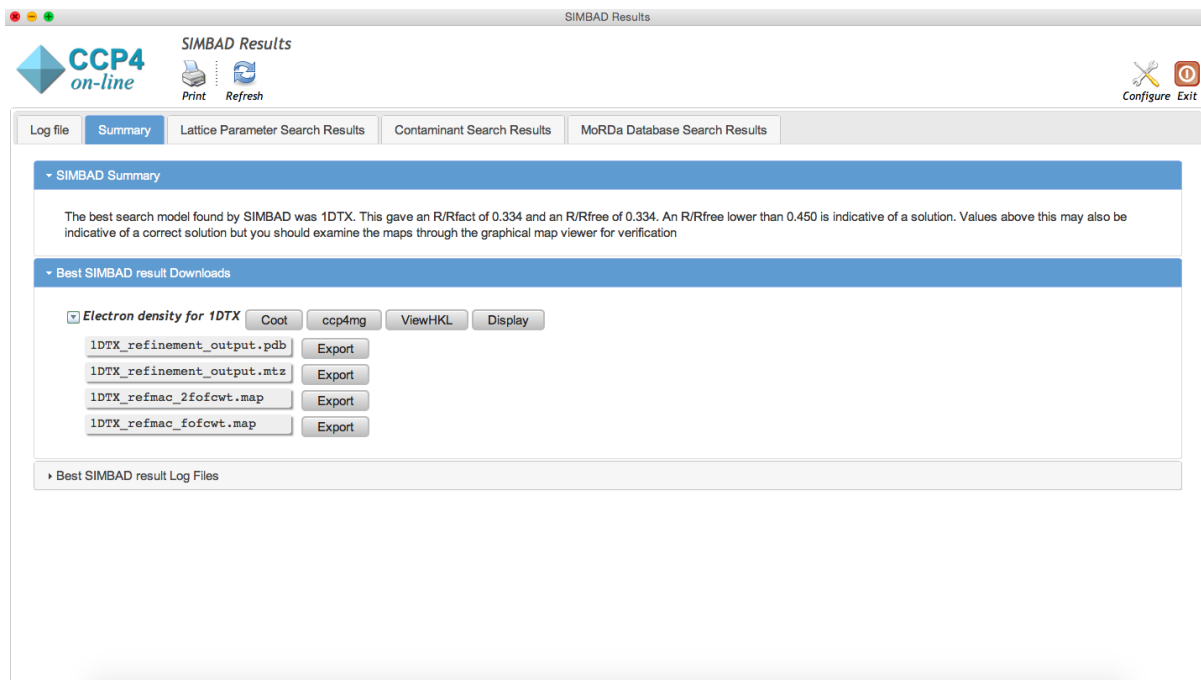
STRUCTURAL
BIOLOGY

Volume 74 (2018)

Supporting information for article:

***SIMBAD*: a sequence-independent molecular-replacement pipeline**

Adam J. Simpkin, Felix Simkovic, Jens M. H. Thomas, Martin Savko, Andrey Lebedev, Ville Uski, Charles Ballard, Marcin Wojdyr, Rui Wu, Ruslan Sanishvili, Yibin Xu, María-Natalia Lisa, Alejandro Buschiazso, William Shepard, Daniel J. Rigden and Ronan Keegan



The screenshot displays the SIMBAD Results web interface. At the top, the CCP4 on-line logo is visible on the left, and the title "SIMBAD Results" is centered. On the right, there are icons for "Print", "Refresh", "Configure", and "Exit". Below the header, a navigation bar contains tabs for "Log file", "Summary", "Lattice Parameter Search Results", "Contaminant Search Results", and "MoRDa Database Search Results". The "Summary" tab is selected and highlighted in blue. The main content area is divided into sections:

- SIMBAD Summary:** A blue header bar followed by a text box stating: "The best search model found by SIMBAD was 1DTX. This gave an R/Rfact of 0.334 and an R/Rfree of 0.334. An R/Rfree lower than 0.450 is indicative of a solution. Values above this may also be indicative of a correct solution but you should examine the maps through the graphical map viewer for verification".
- Best SIMBAD result Downloads:** A blue header bar followed by a section titled "Electron density for 1DTX" with a dropdown arrow. Below this are four buttons: "Coot", "ccp4mg", "ViewHKL", and "Display". Underneath are four rows of file names with "Export" buttons:
 - 1DTX_refinement_output.pdb
 - 1DTX_refinement_output.mtz
 - 1DTX_refmac_2fofcwt.map
 - 1DTX_refmac_fofcwt.map
- Best SIMBAD result Log Files:** A section with a right-pointing arrow and the text "Best SIMBAD result Log Files".

Figure S1 A SIMBAD report page showing a summary tab from a SIMBAD run.