



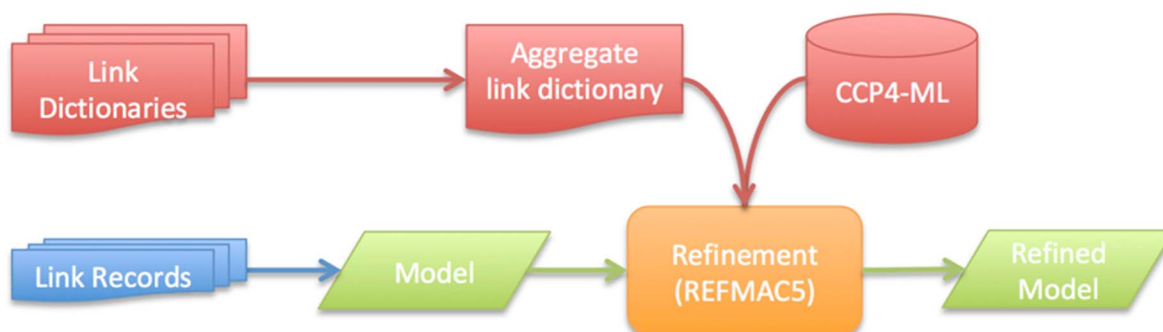
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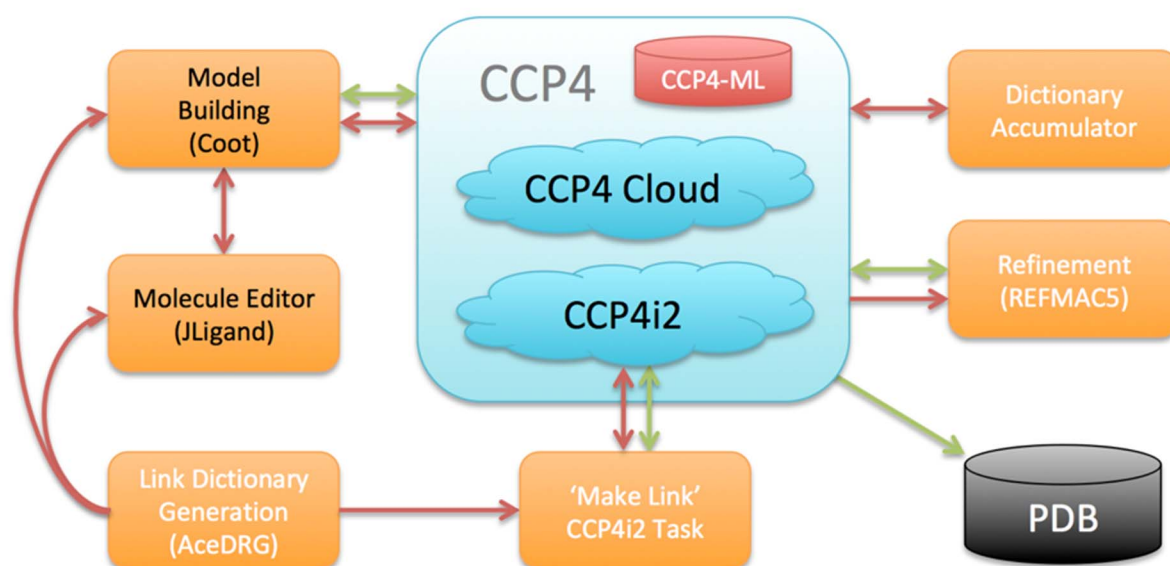
**Supporting information for article:**

### **Modelling covalent linkages in *CCP4***

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**Figure S1** Linkage information dataflow in *CCP4*, focussing on the application of refinement with *REFMAC5*. The refinement process is depicted as an orange rectangle, data are represented as document symbols (arrays indicate potential presence of multiple instances), models as parallelograms, and the CCP4-ML databank as a cylinder. Arrows indicate directional flow, coloured according to the matching data type – red for link dictionaries, blue for link records, and green for models.



**Figure S2** *CCP4* GUI-centric linkage process flow diagram. Processes are depicted as orange rectangles, databanks as cylinders, and GUIs as blue clouds. Arrows indicate directional flow, coloured according to the matching data type – red for link dictionaries, and green for models. Text labels are coloured black for graphical interactive processes, and white for (semi-)automated processes and data.