

Archiving files related to finalized structures

For potential validation and truncation analysis, especially regarding the CC*/CCWORK/CCFREE comparison https://www.phenix-online.org/documentation/reference/unmerged_data.html

For each dataset

In `\\labo4\projets\cava\PRMTs`

- create a `\PRMTx_ligand_drop_PDBID\` directory
- create `\validation` and `\datacol` sub-directories
- all validation files are placed in the `\validation` sub-directory
- the following files are gathered in the `\datacol` sub-directory
 - necessary files for processing (XDS.INP for XDS, ...)
 - log files from processing (CORRECT.LP for XDS, scale.log for HKL)
 - generated files from processing (XDS_ASCII.HKL for XDS, output.sca for HKL)
 - scaled mtz file with all data and no truncation and the corresponding log file
 - cleaned mtz (truncation, 6 columns only, Rfree flag from reference set) and the corresponding log file
 - necessary files for refinement (.cif, .tls, .eff ...)
 - last refinement files (model pdb file and mtz map file)

From:

<https://bsi.inscog.eu/> - **BSI wiki**

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https://bsi.inscog.eu/doku.php?id=crystallography:deposition:data_storage&rev=1464276283

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