

1 Implementation of Data Processing with XDS

1.1 Indexing

`xycorr -> init -> colspot -> idxref -> [select] -> idxref`

1.2 Integration 1

`[select p1] -> defpix -> integrate [-> correct]`

1.3 Pointgroup Determination

`integrate.hkl -> combat -> pointless -> [select indexing solution]`

1.4 Integration 2

`[select indexing solution] -> defpix -> integrate -> correct [in correct pg]
if fail, --spacegroup; repeat`

1.5 Reindexing & Spacegroup Determination

`[sweep 1] -> [quick scale]
[n] * xds_ascii.hkl -> pointless [reindex against quick scale] -> correct`

1.6 Scaling & Merging

`xscale [output unmerged] -> scala`