

# Aimless

```
>setccp4  
>ccp4i
```

Create a project in the /ccp4 subfolder

## Run Aimless

- If XDS was used before, choose the *Option to skip scaling & just merge* to prevent scaling a second time
- If there are several datasets/scans for the same crystal scale and merge all sets in Aimless
- If necessary choose *Customise symmetry determination*>*Choose a previous solution* to force the spacegroup
- If necessary choose *Ensure unique data & add FreeR column...*>*Copy FreeR from another MTZ* to import the FreeR flags from a reference MTZ file
- Specify the *Project*, *Crystal* and *Dataset* names
- Change the output name to **drop\_scaled1.mtz**
- Make a second run in which you specify the high-resolution cut with *Exclude data resolution [ ... ] greater than [ ] Angstroms* and name the output file **drop\_res\_scaled1.mtz**

## Run Sftools

- Use sftools to *delete columns* and remove the 13 unnecessary columns and name the output file **drop\_res\_scaled1\_6col.mtz**
- Use sftools to *delete reflections* and *Delete selected reflections: where Selection includes reflections with data missing in specified column (F\_drop)* and name the output file **drop\_res\_scaled1\_6col\_cleaned.mtz**

From:

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Permanent link:

[https://bsi.inscog.eu/doku.php?id=crystallography:processing:aimless\\_procedure](https://bsi.inscog.eu/doku.php?id=crystallography:processing:aimless_procedure)

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