Supporting information

S1. Currently available options for using *XDSAPP* in the command line mode

The complete list of commands can be invoked by typing `xdsapp --help`

Table S1 List of options for the command line mode of *XDSAPP*, sorted alphabetically.

Option	Shortcut	Description	Example
`--all`	`-a`	Process all data sets found in this folder and all subfolders.	`--all`
`--ccstar`		Do resolution cut-off based on CC*.	`--ccstar`
`--cont`		Look continuously for new data sets in this folder and all subfolders and process them.	
`--cpu`	`-c`	Set the number of processors to be used by *XDS*. If not used, all available CPUs are used, except at the HZB-MX beamlines, as described in the main text of the paper.	`--cpu=4`
`--delphi`		Define the value of DELPHI.	`--delphi=15`
`--dir`		Output folder. By default, the results are output into a subfolder of the images folder.	`--dir=/my/path/`
`--fried`	`-f`	Value for FRIEDEL'S_LAW: true, false or unknown (case insensitive). The default is unknown, meaning that *XDSAPP* will determine it.	`--fried=true`
`--image`	`-i`	If processing only one data set, give the file name of one of its images. The name template will be derived by *XDSAPP*.	`--image=dataset_01_152.img`

`--index`		Only index the given data set.	`--index`
`--jobs`	`-j`	Number of parallel jobs for *XDS*. Default: 3.	`--jobs=1`
`--live`		Enable live processing during data collection. The number of the last expected image is required.	`--live=1500`
`--nice`		Nice level to run *XDS*. Default: 19.	`--nice=10`
`--norestest`		If omitted, a resolution test will be performed for PILATUS data sets prior to integration.	`--norestest`
`--org`		Give the values for ORGX and ORGY.	`--org="1224 1250"`
`--polar`		POLARIZATION_PLANE_NORMAL. Default: 0 1 0.	`--polar="0 1 0"`
`--range`		Range of images to be processed	`--range="1 1200"`
`--raxis`		Values for ROTATION_AXIS. Default: 1 0 0.	`--raxis="1 0 0"`
`--res`		Resolution limit of the data set.	`--res=1.25`
`--reint`	`-r`	Maximum number of smart reintegration cycles to be performed. Default: 3.	`--reint=2`
`--spacegroup`	`-s`	Give the space group number and cell parameters.	`--spacegroup="96 78 78 37 90 90 90"`
`--spotrange`		Values for SPOT_RANGE. Image ranges to be used by *COLSPOT*.	`--spotrange="1 10 20 40 60 80"`
`--suffix`		Give the suffix of your images.	`--suffix=.cbf`
`--xaxis`		DIRECTION_OF_DETECTOR_X-AXIS. Default: 1 0 0.	`--xaxis="1 0 0"`
`--xdsinp`		Generate the file XDS.INP for this data set.	`--xdsinp`
`--yaxis`		DIRECTION_OF_DETECTOR_Y-AXIS. Default: 0 1 0.	`--yaxis="0 1 0"`