

pipedream reference card

most useful options

Brief help message	pipedream
Print autoproc buster rhofit help	pipedream -h process refine rhofit
Simple run, starting from unprocessed images	pipedream -imagedir dir -xyzin pdbfile -hklref mtzfile -d outputdir
Simple run, starting from specified scan of images	pipedream -imagescan <idN>,<dirN>,<templateN>,<fromN>,<toN> -xyzin pdbfile -hklref mtzfile -d outputdir
Simple run starting from pre-processed mtz file	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -d outputdir
No reference mtz file input	pipedream -hklin mtzfile -xyzin pdbfile -nofreeref -d outputdir
Explicitly define direct beam position for autoPROC	pipedream -imagedir dir -beam "153.2 158.4" -xyzin pdbfile -hklref mtzfile -d outputdir
Test all transformation possibilities of direct beam position in autoPROC	pipedream -imagedir dir -beaminitt -xyzin pdbfile -hklref mtzfile -d outputdir
Use autoPROC macro in processing	pipedream -imagedir dir -mproc macroname -xyzin pdbfile -hklref mtzfile -d outputdir
Specify chains or groups of chains to be treated as separate bodies in the limited MR step	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -chains "AB C D" -d outputdir
Use "quick" refinement protocol	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -quick -d outputdir
Use buster macro in refinement	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -mrefine macroname -d outputdir
Define restraint dictionaries for ligands present in the reference structure	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -l dict1,dict2,dict3... -d outputdir
Run rhofit to fit a single ligand	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -rhofit dict -d outputdir
Run rhofit to fit a cocktail of ligands	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -rhofit dict1,dict2,dict3... -d outputdir
Define number of "binding sites" for rhofit to fit to	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -rhofit dict -xclusters <n> -d outputdir
Post-refine best rhofit solution – default protocol	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -rhofit dict -postref -d outputdir
Post-refine best rhofit solution – quick protocol	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -rhofit dict -postquick -d outputdir
Reference mtz file DOES NOT contain FreeR flags	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -nofreeref -d outputdir
Retain water structure present in the input model	pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -keepwater -d outputdir

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Restrict number of “processors” that pipedream process can use	<code>pipedream -hklin mtzfile -xyzin pdbfile -hklref mtzfile -nthreads <n> -d outputdir</code>
Run with pre-processed mtz file and multiple input models. Automatically determine differences between input models	<code>pipedream -hklin mtzfile -xyzin pdbfile1,pdbfile2,pdbfile3 -hklref mtzfile1 -d outputdir</code>
As above, but specify list of residues to use for comparison from input file	<code>pipedream -hklin mtzfile -xyzin pdbfile1,pdbfile2,pdbfile3 -hklref mtzfile1 -seqin1 residues.list -d outputdir</code>
As above, but specify list of residues to use for comparison on command line	<code>pipedream -hklin mtzfile -xyzin pdbfile1,pdbfile2,pdbfile3 -hklref mtzfile1 -seqin2 “ALA A 23,GLY A 24,THR A 25” -d outputdir</code>
Use anisotropically scaled output from Staraniso as input to all subsequent refinement steps	<code>pipedream -imagedir <dir> -xyzin pdbfile -hklref mtzfile -useaniso</code>
Run SideAide (PDB_REDO) to refit incorrectly modelled sidechains by rotamer search	<code>pipedream -hklin mtzfile -xyzin pdbfile -remediate -d outputdir</code>
In addition, allow SideAide to rebuild stubbed residues	<code>pipedream -hklin mtzfile -xyzin pdbfile -remediate -sidechainrebuild -d outputdir</code>
In addition to SideAide, also run pepflip to check for and correct peptide bond flips	<code>pipedream -hklin mtzfile -xyzin pdbfile -remediate -runpepflip -d outputdir</code>