BIOLOGICAL
CRYSTALLOGRAPHY

Volume 71 (2015)

Supporting information for article:

REdiii: a pipeline for automated structure solution

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Table S1 Preset parameters for tools used by *REdiii*. Parameters which were forwarded to the respective tool for the presented test cases. Values in brackets can be optionally set by the user and were not predefined in the test cases.

Indexing (*Xia2*)	project name	crystal name	(space group)	(resolution)	additional options: -3daii			
Molecular Replacement (*AutoMR/BALBES*)	project name	crystal name	search model	(rms) default is 1	mass	copy number	reflection file	additional options *AutoMR*: nproc=5 build=False
Model Building (*AutoBuild/ARP wARP/Buccaneer*)	project name	crystal name	starting model	reflection file	sequence file	additional options *AutoBuild*: nproc=5, build_type=RESOLVE	additional options *ARP/wARP*: fp {F} sigfp {SIGF} freelabin {FreeR_flag}	
Ligand Fitting (*phenix.ligandfit*)	project name	crystal name	starting model	ligand geometry	reflection file	additional options: nproc=2 ordered_solvent=true refinement.input.xray_data.labels=IMEAN,SIGIMEAN		