BUSTER reference card

set up	
Set up for csh or tcsh	**source /some/where/buster/installed/setup.csh**
Set up for sh, bash, ksh, or dash	**. /some/where/buster/installed/setup.sh**
Check all 3rd party tools used by BUSTER work	**checkdeps**
Download PDB entry (code 1abc) and convert SF to mtz	**fetch_PDB 1abc**
BUSTER refinement most useful options	
Brief help message	**refine -h**
Default refinement: **long** 5 big cycles * 100 small cycles	**refine -p protein.pdb -m reflects.mtz ** **-d res.dir > results.log**
No refinement, just maps	refine -p pdb -m mtz -d dir **-M MapOnly** > log
Quick refine (after coot rebuild)	refine -p pdb -m mtz -d dir **-M ShortRunVoid** > log
Medium length refinement	refine -p pdb -m mtz -d dir **-nbig 2** > log
Use NCS restraints (LSSR)	refine -p pdb -m mtz -d dir **-autoncs** > log
TLS basic mode	refine -p pdb -m mtz -d dir **-M TLSbasic** > log
Ligand dictionary (see below)	refine -p pdb -m mtz -d dir **-l grade-XXX.cif** > log
Use QM method for ligand LIG	refine -p pdb -m mtz -d dir **-l grade-LIG.cif -qm LIG** \\ > log
Rigid body for first big cycle	refine -p pdb -m mtz -d dir **-RB** > log
Water updating	refine -p pdb -m mtz -d dir **-WAT** > log
Target restraints (LSSR) to a reference structure	refine -p pdb -m mtz -d dir **-target high_res.pdb** > log
Occupancy refinement	**pdb2occ -p pdb -o pdb-occ.Gelly** refine -p pdb -m mtz -d dir **-Gelly pdb-occ.Gelly** > log
Find ligand binding sites for rhofit	refine -p pdb -m mtz -d dir **-L** > log
Add hydrogen atoms to protein and its ligand, then refine. Use at better than 2.0Å resolution	**hydrogenate -p prot.pdb -l grade-XXX.cif -o protH.pdb** refine **-p protH.pdb** -m mtz -d dir -l grade-XXX.cif > log
An example: initial very long refinement of molecular replacement solution	**refine -p MR.pdb -m refl.mtz -d res.dir ** **-RB -target MR.pdb -nbig 10 > results.log**
Looking at BUSTER refinement results	
Produce report on **refine** run	**buster-report -d dir**
view buster-report output	**firefox dir-report/index.html**
Start **coot** to see structure with maps plus "unhappy atoms" list	**visualise-geometry-coot res.dir**

For latest version of BUSTER reference card see file **$BDG_home/docs/buster_reference_card.pdf**

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BUSTER reference card **cif restraint dictionary preparation**	
Brief help message	**grade -h** and **grade_PDB_ligand -h**
SMILES residue name LIG note: use of **' '**	**grade -resname LIG 'C1CN(CCN1CCO)CCS(=O)(=O)O'**
From mol2 file (with hydrogen atoms)	grade **-in ligand.mol2** -resname LIG
Charged ligand	grade -in acid.mol2 -resname LIG **-charge -1**
Ligand exists in PDB eg 3AS	**grade_PDB_ligand 3AS**
Examine (and edit) cif dictionary	**EditREFMAC grade-LIG.cif grade-CUF.pdb LIG**
Ligand fitting	
Brief help message	**rhofit -h**
Fit ligand XXX	**rhofit -p protein.pdb -m refine.mtz -l grade-XXX.cif \ -d rhofit.dir**
Fit ligand in 2 sites	rhofit -p prot.pdb -m mtz -l cif -d dir **-xclusters 2**
Allow chiral centres to invert during fit	rhofit -p prot.pdb -m mtz -l cif -d dir **-nochirals**
Look at **rhofit** results using **coot**	**cd rhofit.dir** **visualise-rhofit-coot**
refine from rhofit best fits in each site (use with caution!)	**refine -p rhofit.dir/merged.pdb** \ **-l rhofit.dir/best.cif** -m mtz -autoncs > log
Other tools	
Calculate an anomalous Fourier map	**diff_fourier -m truncate.mtz -p refine.mtz \ -P PH2FOFCWT FOM**
Calculate a Fo-Fo differenec Fourier map (and compare positive peaks to PDB file)	diff_fourier **-m apo.mtz -m2 inhibitor.mtz \ -p apo_refine.mtz** -P PH2FOFCWT FOM \ -o Fo-Fo -noANO \ **-pdb apo_refine.pdb**
Calculate an early-late difference Fourier map (and compare within 3Å to PDB file)	diff_fourier **-m late.mtz -m2 early.mtz \ -p refine.mtz** -P PH2FOFCWT FOM \ -o early-late -noANO \ **-pdb refine.pdb -compare_cut 3.0**

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