

BUSTER reference card	
set up (if not already done for you automatically)	
Set up for csh or tcsh	<code>source /some/where/buster/installed/setup.csh</code>
Set up for sh, bash, ksh, or dash	<code>./some/where/buster/installed/setup.sh</code>
Check if all 3rd party tools used by BUSTER work	<code>checkdeps</code>
Download PDB entry (code 1abc) and convert SF to MTZ	<code>fetch_PDB 1abc</code>
BUSTER refinement most useful options	
Brief help message	<code>refine -h</code>
Defining output directory and saving standard output (multiple possibilities)	<code>refine ... -d <output> > output.log 2>&1 # bash</code> <code>refine ... -d <output> >& output.log # (t)csh</code> <code>refine ... -d <output> tee output.log</code>
Default refinement: long 5 big cycles * 100 small cycles	<code>refine -p protein.pdb -m reflects.mtz \</code> <code>-d res.dir > results.log</code>
No refinement, just maps	<code>refine -p pdb -m mtz -d dir -M MapOnly > log</code>
Quick refine (after coot rebuild)	<code>refine -p pdb -m mtz -d dir -M ShortRunVoid > log</code>
Medium length refinement	<code>refine -p pdb -m mtz -d dir -nbig 2 > log</code>
Use NCS restraints (LSSR)	<code>refine -p pdb -m mtz -d dir -autoncs > log</code>
TLS basic mode	<code>refine -p pdb -m mtz -d dir -M TLSbasic > log</code>
Ligand dictionary (see below)	<code>refine -p pdb -m mtz -d dir -l grade-XXX.cif > log</code>
Use QM method for ligand LIG	<code>refine -p pdb -m mtz -d dir -l grade-LIG.cif -qm LIG \</code> <code>> log</code>
Rigid body for first big cycle	<code>refine -p pdb -m mtz -d dir -RB > log</code>
Water updating	<code>refine -p pdb -m mtz -d dir -M WaterUpdatePkmaps > log</code>
Target restraints (LSSR) to a reference structure	<code>refine -p pdb -m mtz -d dir -target high_res.pdb > log</code>
Occupancy refinement	<code>pdb2occ -p pdb -o pdb-occ.Gelly</code> <code>refine -p pdb -m mtz -d dir -Gelly pdb-occ.Gelly > log</code>
Assess possible ligand binding and find ligand binding site(s)	<code>refine -p pdb -m mtz -d dir -L > log</code>
Add hydrogen atoms to protein and its ligand, then refine. Use at better than 2.0Å resolution	<code>hydrogenate -p prot.pdb -l grade-XXX.cif -o proth.pdb</code> <code>refine -p proth.pdb -m mtz -d dir -l grade-XXX.cif > log</code>
An example: initial very long refinement of molecular replacement solution	<code>refine -p MR.pdb -m refl.mtz -d res.dir \</code> <code>-RB -target MR.pdb -nbig 10 > results.log</code>
Looking at BUSTER refinement results	
Produce report on refine run	<code>buster-report -d dir</code>
view buster-report output	<code>firefox dir-report/index.html</code>
Start coot to see structure with maps plus “unhappy atoms” list	<code>visualise-geometry-coot res.dir</code>
Use coot for displaying final BUSTER model and maps	<code>cd res.dir</code> <code>coot -pdb refine.pdb -auto refine.mtz</code>

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

BUSTER reference card	
cif restraint dictionary preparation	
Brief help messages	grade -h grade_PDB_ligand -h
SMILES residue name LIG (use single quotes '...')	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 difference 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
Further documentation and resources	
Global Phasing home page	http://www.globalphasing.com/
Grade (restraint dictionary generator) web service	http://grade.globalphasing.org/
BUSTER Wiki	http://www.globalphasing.com/buster/wiki/
buster-discuss mailing list	https://www.globalphasing.com/mailman/listinfo/buster-discuss

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