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#!/bin/bash

# prepare Amber and structure factor files needed for xray3-style calculations.
# Single input is the pdb-identifier: code assumes that $1-sf.cif
# and $1.pdb are available in the current directory

id=$1
echo "XrayPrep log file for id $id" > $id-prep.log

#####
echo "Running phenix.AmberPrep"
phenix.AmberPrep $id.pdb >> $id-prep.log \
  || { echo " phenix.AmberPrep: Program error"; exit 1; }

# next only needed for ions: how to automate?
perl -pi -e 's/CL$/CL-1/' ${id}_uc.pdb \
  || { echo " perl: Program error"; exit 1; }

echo "creating ${id}_uc.parm7"
/bin/rm -f ${id}_uc.parm7
add_pdb -i 4amber_${id}.prmtop -p ${id}_uc.pdb -o foo.parm7 >> $id-prep.log \
  || { echo " add_pdb: Program error"; exit 1; }
add_xray -i foo.parm7 -o foo2.parm7 >> $id-prep.log \
  || { echo " add_xray: Program error"; exit 1; }
parmed -n <<EOF >> $id-prep.log \
  || { echo " parmed: Program error"; exit 1; }
parm foo2.parm7
lmod
parmout ${id}_uc.parm7
go
EOF

/bin/mv 4amber_${id}.rst7 ${id}_uc.rst7

#####
echo "Expanding reflections to P1 symmetry"

phenix.reflection_file_converter cdl_001.mtz --expand_to_p1 \
  --label="F-obs-filtered.SIGF-obs-filtered" --generate_r_free_flags \
  --r_free_flags_format=ccp4 --mtz=${id}-P1.mtz >> $id-prep.log

#####
echo "Making the sf.dat file"
# convert to formatted file:
phenix.mtz.dump -c -f s ${id}-P1.mtz | tr ',' '\t' > $id.fmtz \
  || { echo " phenix.mtz.dump: Program error"; exit 1; }

# make the -sf.dat file needed by xray3:
awk '{printf("%d\t%d\t%d\t%s\t%s\t%d\n",\
  $1,$2,$3,$4,$5,$6>1?1:$6)}' $id.fmtz | tail +2 > tmp.dat \
  || { echo " awk: Program error"; exit 1; }

nrefl='wc -l tmp.dat | awk '{print $1}''
echo "$nrefl 0" > $id-sf.dat
cat tmp.dat >> $id-sf.dat

#####
echo "Done. Created 5 files:"
echo "  ${id}_uc.parm7      Use this as the Amber prmtop file"
echo "  ${id}_uc.rst7       Starting coordinates in Amber restrt format"
echo "  ${id}_uc.pdb         Use as pdb_infile"
echo "  ${id}-sf.dat         Use as reflections_infile"
echo "  ${id}-prep.log       Log file: examine this if problems arise"

#####
# clean up
/bin/rm -f tmp.dat $id-sf.mtz cdl_data.mtz $id-P1.mtz $id.fmtz \
  cdl_00* *.order 4phenix_${id}.pdb 4amber_480d.prmtop foo.parm7 foo2.parm7

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