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<pre> import sys import iotbx.mtz sys.path.append("/Users/kuntaro/00.Develop/Prog/02.Python/Libs/") from ReflWidthBothEdge import * # Take common reflections def commonalize(*Is): new_Is = [] Is0 = Is[0] for I in Is[1:]: Is0, I = Is0.common_sets(I, assert_is_similar_symmetry=False) new_Is.append(I) Is = [] for I in new_Is: I = I.common_set(Is0, assert_is_similar_symmetry=False) assert len(Is0.data()) == len(I.data()) Is.append(I) return [Is0,] + Is # commonalize() # One liner function for extracting Intensity related columns in MTZ file get_I_arrays = lambda x: filter(lambda y: y.is_xray_intensity_array(), x) #def run(ref_mtz, frame_mtz, matfile, tbatch, pthresh): def run(ref_mtz, frame_mtz, matfile, tbatch, pthresh, mosaic, phistep): # MTZ file reading ref_arrays = iotbx.mtz.object(ref_mtz).as_miller_arrays() frame_arrays = iotbx.mtz.object(frame_mtz).as_miller_arrays(merge_equiva lents=False) # Obtain all of the symmetry operation from FRAME MTZ ops = [op.inverse().r() for op in iotbx.mtz.object(frame_mtz).space_grou p().all_ops()] # Extract intensity related cctbx.array ref_I = get_I_arrays(ref_arrays)[0] frame_I = get_I_arrays(frame_arrays)[0] # Extract M/ISYM m_isym = filter(lambda a: "M_ISYM" in a.info().labels, frame_arrays) [0] # Extract FRACTIONCALC fracc = filter(lambda a: "FRACTIONCALC" in a.info().labels, frame_arrays)[0] sel=fracc.data() > pthresh fracc = fracc.select(sel) # Extract BATCH number batch = filter(lambda a: "BATCH" in a.info().labels, frame_arrays)[0] sel= batch.data()==tbatch batch = batch.select(sel) print "ORIGINAL ref I:", ref_mtz, ref_I.info().label_string(),len(ref_I.da ta()) print "ORIGINAL frm I:", frame_mtz, frame_I.info().label_string(),len(fram e_I.data()) print "ORIGINAL M/ISYM:", frame_mtz, m_isym.info().label_string(),len(m_ isym.data()) # Take common sets of these batch,ref_I,frame_I,m_isym,fracc = commonalize(batch,ref_I,frame_I,m_isy m,fracc) assert len(ref_I.data()) == len(frame_I.data()) == len(m_isym.data()) == len(fracc.data()) print "CHOSEN ref I:", len(ref_I.data()) print "CHOSEN frm I:", len(frame_I.data()) </pre>		

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<pre> print "CHOSEN M/ISYM:", len(m_isym.data()) # delete FULL/PARTIAL flag isyms = m_isym.data()%256 # scale factor scale=1.0 tmp=frame_I.customized_copy(data=frame_I.data()*scale) # Preparation for diffraction width rwbe=ReflWidthBothEdge(matfile,0.02,0.02,mosaic,0.0002,phistep) for (hkl1,rI,rsigI),(hkl2,fI,fsigI),isym,frac in zip(ref_I,tmp,isyms,frac c.data()): assert hkl1 == hkl2 # Calculate original index sign = -1 if isym%2 == 0 else 1 ohkl = hkl1*ops[int((isym-1)/2)] ohkl = tuple(map(lambda x:int(x*sign), ohkl)) h=ohkl[0] k=ohkl[1] l=ohkl[2] pobs=fI/rI phi=0.1*float(tbatch-1) rwbe.setHKL(ohkl,0.0) rwbe.calcDELEPS() pcalc=rwbe.calcPartiality() print "%5d%5d%5d%12.1f%12.1f%12.7f%12.7f%12.7f"% (h,k,l,rI,fI,pobs,frac,pcalc) #print hkl1,ohkl,rI,fI print "Done." if __name__ == "__main__": if len(sys.argv)!=7: print "REFMTZ FRAMEMTZ MATFILE BATCH PTHRESH MOSAIC OSCSTEP" ref_mtz = sys.argv[1] frame_mtz = sys.argv[2] mat_file=sys.argv[3] batch=int(sys.argv[4]) pthresh=float(sys.argv[5]) mosaic=float(sys.argv[6]) phistep=float(sys.argv[7]) run(ref_mtz, frame_mtz, mat_file, batch, pthresh, mosaic, phistep) </pre>		