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|--|--|----------|
| import os, sys import iotbx.mtz | | |
| class ReadMtz: | | |
| def __init__(self, mtzfile, merge_option=False): | self.mtz=mtzfile self.isInit=False self.isMerge=merge_option self.isSymm=False | |
| def init(self): | self.m=iotbx.mtz.object(self.mtz) if self.isMerge: self.arrays=self.m.as_miller_arrays() else: self.arrays=self.m.as_miller_arrays(merge_equivalents=Fa | |
| lse) | | |
| def showSummary(self): | if self.isInit==False: self.init() self.m.show_summary() | |
| def getIntensityArray(self): | if self.isInit==False: self.init() | |
| ray(), x) | # yam-god function get_I_arrays = lambda x: filter(lambda y: y.is_xray_intensity_ar | |
| | self.i_related=get_I_arrays(self.arrays)[0] return self.i_related | |
| def getIoverZero(self): | self.I_ok=self.getIntensityArray() self.I_ok=self.I_ok.select(self.I_ok.data()>0.0) return self.I_ok | |
| hresh) | def getReliableI(self, thresh=2.0): self.I_ok=self.getIntensityArray() norig=len(self.I_ok.data()) print "ORIG:%5d"%norig self.I_ok=self.I_ok.select(self.I_ok.data()>0.0) nsele=len(self.I_ok.data()) print "I>0.0:%5d"%nsele self.I_ok=self.I_ok.select(self.I_ok.data()/self.I_ok.sigmas()>t | |
| | nsele=len(self.I_ok.data()) print "I/sig>%5.2f:%5d"%(thresh, nsele) #for d in self.I_ok.data(): #print d #print norig, nsele return self.I_ok | |
| | def getColumn(self, colname): if self.isInit==False: self.init() obje=filter(lambda a: colname in a.info().labels, self.arrays)[0] return obje | |
| | def getSymmOption(self): if self.isInit==False: self.init() self.ops = [op.inverse().r() for op in self.m.space_group().all_ | |
| ops()) | | |

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|----------------|---|----------|
| | self.isSymm=True return self.ops | |
| | def getOriginalIndex(self, hkl, isym): if self.isSymm!=True: self.getSymmOption() # Calculate original index sign = -1 if isym%2 == 0 else 1 ohkl = hkl*self.ops[int((isym-1)/2)] ohkl = tuple(map(lambda x: int(x*sign), ohkl)) return ohkl | |
| | # Take common reflections def commonInfo(self, *Is): new_Is = [] Is0 = Is[0] for I in Is[1:]: Is0, I = Is0.common_sets(I, assert_is_similar_symmetry=F | |
| alse) | 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 | |
| | if __name__=="__main__": filename=sys.argv[1] m=ReadMtz(filename) #m.showSummary() #print m.getSymmOption() fracc=m.getColumn("FRACTIONCALC") batch=m.getColumn("BATCH") m_isym=m.getColumn("M_ISYM") fracc, batch, m_isym=m.commonInfo(fracc, batch, m_isym) #print m.getMillerOrig() #print m.getRealFlex("FRACTIONCALC") | |