2dx_merge, Version 2dx-3.4.1

Difference Map

Standard Scripts

- Initialization
- Merge Once
- Refine Once
- Merge & Refine (Iterati... 3
- Generate Image Maps
- Final Merge
- Generate Merged Map
- (Re-)Process all images

Custom Scripts

- Calculate Ideal Dataset
- Image Inventory
- Merge with Custom Inp...
- Cleanup
- Difference Map
- Synchronize Project wit...
- Backup Databases
- Delete Images
- Prepare Large Images (e...

Image Preview

No Image Selected

/Users/crpaulin/Documents/Workshops&Conferences/2dx_Workshop2012/DiffMap-Workshop/merge/

Processing Data -- Advanced

Lattice Determination		
Real Unit Cell Length (for entire project): 1	80	108
Real Cell Angle (for entire project):	90.0	
Common Image Processing		
Lower Resolution Limit (RESMIN): 2	200.0	
Upper Resolution Limit (RESMAX):	8	
Plot generation		
Contour and step size for the map generation: 6	*0.6*	
Contour threshold for the map generation: 5	*0*	
Difference Map		
projection map 1:	Path for Map1.mtz	
name of map 1: 3	Map1	
projection map 2:	Path for Map2.mtz	
name of map 2:	Map2.mtz	
Contour mode: 4	SIG	
Mibimum contour level for the dfifference map generation: 5	-3.0	
Maximum contour level for the dfifference map generation:	3.0	
Contour and step size for the dfifference map generation: 6	0.5	

Logfile - Low Verbosity

```
==== Limiting the resolution to 8 ==========================================
==== Inverse fft to get map ================================================
==== npo - to create a line plot for both maps =============================
==== laserplot - to create PS/4D1.ps =======================================
==== npo - to plot the overlay =============================================
==== laserplot - to create PS/4D1_4D2_overlay.ps ===========================
==== overlapmap -  to calulate difference map - 4D1 - 4D2 ==================
==== npo - to create a line plot for difference map ========================
==== laserplot - to create  PS/diff_map1_4D1-diff_map2_4D2_diffmap.ps ======
==== npo - to create a line plot for map 1 & difference map ================
```

Results

Parameter	Value

Images

- MTZ: Map 1 with scaled amplitudes
- MTZ: Map 2 with scaled amplitudes
- MTZ: Map 1 (resolution limited)
- MTZ: Map 2 (resolution limited)
- PS: map 1
- PS: map 2
- PS: overlay of both maps 7
- PS: Difference Map
- Map 1 and Difference Map