

JCSG Data Collection

http://sdc08.slac.stanford.edu:3000/collection/edit/16297

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Editing Data

HP10645F 137473_2 [Show](#) | [Collection List](#) | [Delete](#) | [Xsolve](#) | [Xsolve Upload](#) | [Processing Results](#)


Date Data Collected:	2009-12-04		
Beamline:	BL11_1		
Target:	HP10645F		
Crystal ID:	137473_2		
Experiment:	SAD		
Resolution:	2.1		
Data Collected by:	Jessica		
Image Directory:	/data/jcsg/ssrl4/11_1/20091202/collection/HP10645F/137473		
HKL2000 Spotsize:			
Autoindex Images:	Prefix:	Image1:	Image2:
Beam Center:	BeamX:	BeamY:	
Lambda1:	fp: -7.2695	fpp: 5.2442	prefix list: 137473_1
Lambda2:	fp:	fpp:	prefix list:
Lambda3:	fp:	fpp:	prefix list:
Lambda4:	fp:	fpp:	prefix list:
Space Group List:	P1		
Number of Molecules:			
Comments:	<pre> 04 Dec 2009 10:59:22 AM stog_operation_completed madScan 46.175 normal 12657.330078 -9.360322 3.041869 12663.870117 -7.269518 5.244236 13500.000000 - 1.800000 3.400000 NULL/137473scan 137473smooth_exp.bip 137473smooth_norm.bip 137473fp_fpp.bip 04 Dec 2009 10:59:22 AM Inflection Energy: 12657.330078 eV 04 Dec 2009 10:59:22 AM Inflection f' : -9.360322 04 Dec 2009 10:59:22 AM Inflection f'' : 3.041869 </pre>		

Xsolve - Automatic Struc... x

http://sdc64.slac.stanford.edu:8080/jcsg/xsolve.jsp?user=jcsg&dataid=16297

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[Data Collection List](#) [Data Collection Form](#) [Data Processing Form](#) [Upload Xsolve Solution](#)



Xsolve - Automatic Structure Solution

Dataset HP10645F 137473_2

Processing Data: /data/jcsg/xtal_process5/HP10645F/137473_2
 Images: /data/jcsg/ssrl4/11_1/20091202/collection/HP10645F/137473
 Please make sure the [Dataset](#) information is correct before starting the processing.

Start MAD/SAD or Native Processing (for Molecular Replacement click [here](#))

Processing Steps **Strategy (program combination)**

Get Dataset Information (image directory, target...)
 Index + Refine Cell
 Integrate Mosflm HKL2000 XDS
 Scale
 Truncate
 Phasing Solve Sharp
 Model building Buccaneer ARP/wARP Resolve

Xsolve will do **nothing** if you check only the three checkboxes in the last row!
 For more information see the online [help](#).

Status

Sun Dec 27 11:14:48 PST 2009

Target	CrystalID	UserName	HostName	PID	TaskID	TimeStamp	Status
null	null	jcsg	sdc02	26556		Sun Dec 27 11:14:36 PST 2009	wait
null	null	jcsg	sdc03	22688		Sun Dec 27 11:14:44 PST 2009	wait
null	null	jcsg	sdc04	22751		Sun Dec 27 11:14:43 PST 2009	wait
null	null	jcsg	sdc05	22754		Sun Dec 27 11:14:50 PST 2009	wait
MI12113B	143152	jcsg	sdc06	22792	xsolve sdc64 040856 46554	Sun Dec 06 21:22:09 PST 2009	running <input type="button" value="Abort"/>

Xsolve Status

file:///C:/Users/vdbedem/Documents/Meetings/CCP4_2010/Xsolve%20Status.htm

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BUCCANEER (model_buccaneer_sharp)
 Started: Thu Dec 24 03:10:22 PST 2009 Finished: Thu Dec 24 03:10:26 PST 2009
 /data/jcsg/xtal_process5/MG10938A/89622/try1/model_buccaneer_sharp/buccaneer_list.xml
 SC|Nmol|L|Connect|R|Build|Docked|%
 p1 4 123 null 0.4746 2045 382 18.7
 p1 5 123 null 0.4685 1991 250 12.6

BUCCANEER (model_buccaneer_xds)
 Started: Thu Dec 24 03:10:28 PST 2009 Finished: Thu Dec 24 05:20:05 PST 2009
 /data/jcsg/xtal_process5/MG10938A/89622/try1/model_buccaneer_xds/buccaneer_list.xml
 SC|Nmol|L|Connect|R|Build|Docked|%
 p1 4 123 null 0.4746 2045 382 18.7
 p1 5 123 null 0.4685 1991 250 12.6

BUCCANEER (model_buccaneer_sharp_xds)
 Started: Thu Dec 24 03:11:01 PST 2009 Finished: Thu Dec 24 08:02:17 PST 2009
 /data/jcsg/xtal_process5/MG10938A/89622/try1/model_buccaneer_sharp_xds/buccaneer_list.xml
 SC|Nmol|L|Connect|R|Build|Docked|%
 p1 4 123 null 0.2528 2601 2532 97.3
 p1 5 123 null 0.2506 2612 2551 97.7
 p1 7 123 null 0.2316 2622 2580 98.4
 p1 8 23 null 0.4957 1954 271 13.9
 p1 8 123 null 0.2185 2615 2590 99.0

ARP/wARP (model_warp)
 Started: Thu Dec 24 03:12:07 PST 2009 Finished: Thu Dec 24 03:12:11 PST 2009
 /data/jcsg/xtal_process5/MG10938A/89622/try1/model_warp/warp_list.xml
 SC|Nmol|L|Connect|R|Build|Docked|%
 p1 4 123 null 0.273 650 89 13
 p1 5 123 null 0.251 687 82 11

ARP/wARP (model_warp_sharp)
 Started: Thu Dec 24 03:13:13 PST 2009 Finished: Thu Dec 24 03:13:17 PST 2009
 /data/jcsg/xtal_process5/MG10938A/89622/try1/model_warp_sharp/warp_list.xml
 SC|Nmol|L|Connect|R|Build|Docked|%
 p1 4 123 null 0.273 650 89 13
 p1 5 123 null 0.251 687 82 11

ARP/wARP (model_warp_xds)
 Started: Thu Dec 24 03:14:19 PST 2009 Finished: Thu Dec 24 15:25:57 PST 2009
 /data/jcsg/xtal_process5/MG10938A/89622/try1/model_warp_xds/warp_list.xml
 SC|Nmol|L|Connect|R|Build|Docked|%
 p1 4 123 null 0.273 650 89 13
 p1 5 123 null 0.251 687 82 11

ARP/wARP (model_warp_sharp_xds)
 Started: Thu Dec 24 03:15:58 PST 2009 Finished: Thu Dec 24 21:06:35 PST 2009
 /data/jcsg/xtal_process5/MG10938A/89622/try1/model_warp_sharp_xds/warp_list.xml
 SC|Nmol|L|Connect|R|Build|Docked|%
 p1 4 123 null 0.250 1507 955 63
 p1 5 123 null 0.358 1977 1606 81
 p1 7 123 null 0.271 2295 2045 89
 p1 8 23 null 0.228 1627 866 53
 p1 8 123 null 0.261 2341 2218 94

User Interface for Xsolve. The web page at the top gathers information about the experiment. Xsolve is started from a web interface as well, shown in the middle. At the bottom an example of a status page is shown.