CrysAlis^{Pro}: Data reduction different image formats

Mathias Meyer

X-ray Group Software Manager



Copyright © 2016 — Rigaku Corporation and its Global .

Area detector diffraction experiments

- Understand the experiment
- Goniometer description
- Sense of rotation
- Area detector 'perspective'
- Zero points
- Kappa vs. Euler geometry



W. A. Paciorek, M. Meyer and G. Chapuis: 'On the geometry of a modern imaging diffractometer'; Acta Cryst. (1999). A55, 543-557



Copyright © 2016 — Rigaku Corporation and its Global .

Workflow on in-house instruments

- Describe instrument
- Run fully automatic calibration experiment describing fully the instrument at any distance
- Run test data collection on standard sample
- Run new experiment.



Workflow on inhouse instruments Describe instrument

Colluion model (2010, first serv	(GV1000, CC5 camer (es) - port 2500				Dearrando Planciario	I, LACIE INTRACTORE	Trends.
itep 15 - Browse	for name of roachine	folder					
C:Ucalibur\car	rections(Synergy					Second Second	Sectors.
tep 2 · Choose p	platform (machine, so	urce, cettinet) and acc	resories	Thursday	17		
	ShiLAB Serverger	DeetField, MyPle			DCE Pro Atherna	e (2016 - ?] - port 2	511
	Protocolar Cu		Photos Det Mo				
	John .				DistAll Suberga	othinet.	
	Hills carries		٠				
		1.			Station St	Research Street	-
ten 3 - Check for	r files required for Re	alice Oxford Diffraction	VAgient Technologien	instrument setup			
Needed files:	TT.	mil P	- 1		Ignore ".m/#	and/minifit files	100
					If some files are	masing, copy them	to the folder
						0000 < 1000	
					To refresh the fo	NOT - 1000 Adar given in Step 1	and press
Patent	Married Married	Dave In all	these Contra	active house	To refresh the for refresh button	iccos - 1000 Ader grown in Shep 1	and press
tep 4 - Analysis	of Step 3 Riss	Non and a sub			17 To refresh the fr refresh button	inder given in Step 3	and press
tep 5 - Experime	of Step 3 Riss				77 Tu refresh the fr	Aller given in Step 1	Income
tep 1 - Analysis tep 3 - Experime	of Step 3 Riss	Sinet molecule/pr	atter Pitcarner	Saring	12 To refresh the fr refresh buttor,	kie gewin Step 1	
tep 4 - Analysis tep 5 - Experime T	of Step 3 Riss	Snel noleoleje	stere () const Pilling stere Pilling Filling	Saring Saring Saring Saring	12 To refresh buttor.	kor i too kir gan a Sep 1 Pressenter	
tep 1 - Analysis tep 2 - Experiment	of Step 3 Files	Snat redeale/pr	ster PScener	Santa Santa Santa Santa Santa Santa Santa	To refresh buttor.	International	and press
tep 1 - Analysis tep 2 - Experime tep 5 - Experime	of Stage 3 Files	Small moleculator	alaana Canada Maria Canada Maria Canada Maria Canada Maria Canada Maria Canada	Sectors Sectors Francesco	To refresh buttor.	Nove 1000 Alter gave it Step 1 (Nove Alter (Nove Alter) (Nove Alter)	and press
tep 1 - Analysis tep 3 - Experime Tag tep 5 - Moroaco Planmadt WD	of Stage 3 Files	Small molecule/pr (f /// (f /// (A22) • [/fW	alaan (Canada Marina (Canada) Marina (Canada Marina (Canada) Marina (Canada)		To refresh the fire refresh buttor.	Inter Into Alier gave in Step 1 (International International International International International	
tep 1 - Analysis tep 2 - Experime To any 1 - Morrosco Plannack WD tep 2 - Instrume	of Step 3 Riss (n/s) ent personations (n/s) ent personations (n/s) ent personations (n/s)(Small moleculator di (1) (1) (1) (1) (1) (1) (1) (1) (1) (1)	uten Piticarner		12 Tu rehesh the fr rehesh buttor.	1000 - 1000 King gaan is Sop 1 (Transform) (Transform) (Transform)	and press
tep 5 - Experime Top 5 - Experime Top 5 - Herosco Planaat WD tep 7 - Erstrume	of Stap 3 Riss Inte ent personations pervideo settings Pf Jonogo Costure (W) ant personeters	Smell molecularjo (f) (7)	ster Pitterner		12 Tu retresh the fr refresh buttor.		
Esp 1 - Analysis Esp 3 - Experime F top 5 - Horseso Plannack WD top 7 - Instrume	of Step 3 Riss Inte ant personations exervideo unitings If Jonapa Casture (W ant parameters	Small molecule/ye er extra status A123 - WW	alaan ahaa ahaa ahaa ahaa ahaa ahaa ahaa		12 To network the for refresh buttor.		
Social tep 1 - Analysis tep 3 - Experime Ferritary tep 3 - Instrume	of Step 3 Riss Inte ant persovetiers ope video settings If Jonapa Castore (W ett parameters				12 To network the for refresh buttor.		



Workflow on in-house instruments

Run fully automatic calibration experiment describing fully the instrument at any distance

					Full cal	ibration ex	perime	ent diald	og (2.0	.4)		×
Path												
Name:		HyP	ix6000_81016		Browse root folder	C:\Xcalib	urData					
1	ath is ck1	Experim	nent in folder	C:\Xcalib	urData\calib_Hyl	Pix6000_81016_	Sat-Oct-	08-23-07-1	8-2016			
Basic sy Dd zero orientat	stem param (Cu)=-4.000 ion=gemini(eters 100, Dd zero((mkII), HyPix	(Mo)=-4.00000 (1x1 binning,), Overflo Flood co	w threshold=10 rrection: off	48000, Beam st	op suppo	rt		Set	Generator No ch C Turn o C Turn o	r at end of experiment ange down off
Options											Calibratio	n mode
Crystal	Cytidine	•	Lattice type	P-lattic	e 💌	Lattice min	2	max	30	Parameters	Optim Optim Optim	al
User mo	de paramet	ers									C User	4
(salanie)	ets) no con	sustines dan									C Constr	raint
Cu										F a n .		9999 1992 - 1992 - 1997 - 1997 - 1997
Ne	ar	50.00		1.00	Exposure time	the same for a	ll theta p	ositions: 1.	.0s/deg, D	etector distance=	xtra data for bett 39.00, Scan	ter structure refinement
v	kV	50.00	mA	1.00	range=20.0, So	can width=0.1,						Cunear
Fa	r in the second s				Evposure time	the came for a	ll theta n	ositions: 1	Ne/dea D	atactor distances	74.00 Scan	
17 1	kV	50.00	mA	1.00	range=20.0, So	can width=0.1,	n uicto p	0010101101 21	oor degr o	etector distance-	, 1.00, Scan	Cu far
A _s ,	tormatic floo	d field corre	ction calibrati									
Г	Run Tiood		File									
Mo											utra data for bott	ar structure refinament
	kV	50.00	mA	1.00	Exposure time range=10.0, So	the same for a can width=0.1.	ll theta p	ositions: 5.	.0s/deg, D	etector distance=	39.00, Scan	Mo near
Fa	r											
	kV	50.00	mA	1.00	Exposure time range=10.0 Sc	the same for a	ll theta p	ositions: 5.	.0s/deg, D	etector distance=	74.00, Scan	Mo far
- 10	tamatic floa	d Eeld come	ction calibrati	1	runge runo, et	an man ory						
Г	Ran figed		File:									
User me Cytid You I	ssage ine cell: a=! nave change	5.120, b=14.0 d cell type p	000, c=14.800 arameters, vo	, alpha=9 u must re	90.000, beta=90. egenerate calibr	000, gamma=9 ation run lists	0.000 please cli	ck 'Find ex	periment	s' button		
	and change										A	
Find	experiments	End of c	alibration: Sa	t Oct 08 1	23:52:17 2016 (4	H4min)				Help	Start	Exit



Workflow on in-house instruments

Run test data collection on standard sample





Workflow on in-house instruments Run new experiment





Import: Worse situation

- Depending on the format the instrument model is only known so-so.
- Rather than on a ,Standard sample' the import is tried on something difficult.
- ,Easy': Import of known formats
- ,Complex': Esperanto import



- Install CrysAlisPro: this will install a tool called ,CAPFrameView'. You can inspect all known image formats.
- Use of a file inspection program: ,Norton commander'
- A rename tool.







Copyright $\ensuremath{\textcircled{O}}$ 2016 — Rigaku Corporation and its Global .

8		Total Comman	der (x64)	8.50 NICH	IT REGISTRIERT		- 0	×
Dateion Markieren Be	fehle Netz Ansicht Kor	nfigurieren Starter						Hilfe
2 1 2 2 1	5 4 4 4	a a 🚟 🕮 🐽	NEG	5 R				
/ v (data-sid) 323'34	83'288 k von 976'758'780 k f	inui	A	int - Ida	ta-sisd) 323'383'288 k von 97	76'758'780 k frei		A
DCE WinMerne dhol27	binned review 08 Bicaku	include DK ML7-66 MM re		2016 000	e files totalond 01 Projector	mana dhol27 binned ACA Albumur	auton	1.1
+ 120110827 iucr/Eshib	ition Examples/AutochemCr	vsaiisProhdhot27 binned/*.*		+ 1201108	27 jucrExhibition Example	AutochemCrysellePro/dbot27_bing	edit *	
Name		*1	Erw. Größe	4Name			Erw	Größe
\$11			<dir +<="" td=""><td>\$L1</td><td></td><td></td><td></td><td><dir .<="" td=""></dir></td></dir>	\$L1				<dir .<="" td=""></dir>
[frames]			<dir< td=""><td>[frames]</td><td></td><td></td><td></td><td><dir< td=""></dir<></td></dir<>	[frames]				<dir< td=""></dir<>
[log]			<dir< td=""><td>[log]</td><td></td><td></td><td></td><td><dir< td=""></dir<></td></dir<>	[log]				<dir< td=""></dir<>
[sg_dhol27_binned]			<dir< td=""><td>[sg_dhot</td><td>27_binned]</td><td></td><td></td><td><dir< td=""></dir<></td></dir<>	[sg_dhot	27_binned]			<dir< td=""></dir<>
[struct]			<dir< td=""><td>[struct]</td><td>68</td><td></td><td></td><td><dir< td=""></dir<></td></dir<>	[struct]	68			<dir< td=""></dir<>
[tmp]			<dir:< td=""><td>[tmp]</td><td></td><td></td><td></td><td><dir< td=""></dir<></td></dir:<>	[tmp]				<dir< td=""></dir<>
dhol27_binned			ialinfo	a_57_11	1007		geo	1710
a_57_021007		00	d 1'	a 57.02	1007		ccd	11
17137141		cit	4	pre_dhol	27_binned_auto		ini	
dhol27_binned		cit	4	mm3838	mp		ini_n	sport
mm3838		cit	4	mm3838	rint		det	67
17137141		cif	od 4	mm3838	resolutionstats		dat	12
dhol27_binned		cit	od 4	mm3838	refinedsubmodels		det	13'
mms3838		cit	od 4	mm3838	red		sum	65'
1713714t_absscale		da	4 5	mm3838	profiles		dat	6'
1713714t_chi2am		de	r 3'	mm3838	profilecorrres		dat	1
1713714t_chi2bm		da	a 3	mm3838	profilecorriest		det	- T
1713714t_lattice		da	13	mm3838	profilecorrframe		dat	31
1713714t_latticeperrur	1	da	4	mm3838	predictaccuracyvstheta		dat	2
1713714L predictaccur	acyvsframe	da	1 7	mm3838	predictaccuracyvsframecycl	e1	dat	7
17137141 predictaccur	acyvsframecycle1	da	4 7	mm3838	predictaccuracyvsframe		det	7
1713714t_predictaccur	racyvstheta	de	4 2	mm3838	latticeperrun		dat	
1713714t profilecorrfm	ane	da	a 31	mm3838	lattica		det	131
17137141 profilecomm	t	da	a 1'	mm3838	hkl skipregion		tet	1
1713714t_profilecorrre	5	da	1 1	mm3638	hid overflow		tat	
1713714t profiles		da	6 5	mm3838	hki filtered		txt	
1713714t_refinedsubm	odels	da	1 13	mm3838	hkl_edgeskip		txt	10"
1713714t_resolutionsta	ats	da	1 1	mm3838	hkl_badprofile		tet	
1713714t_rint		da	t 6"	mm3838	datared		ini_p	e., 12'
dhol27_binned_abssca	ale	da	4 5	mm3838	crystal		ini_n	up_ 6*
dhol27_binned_bfactor	r.	da	4 5	mm3838	coverage		ini_n	ep. 1'
dhol27_binned_chi2am		da	4 31	mm3838	chi2bm		dat	3
dhol27_binned_chi2bm		da	a 31	mm3838	chi2am		dat	31
dhol27 binned latticep	pernum	de	4	mm3838	absscale		diat	5'
dhot27_binned_maxres		da	8	mm3838			rrppe	rof 904"
dhol27_binned_predict	laccuracyvsframe	da	t 7	mm3838			p4p	
dhol27_binned_profiled	contrame	da	a 3 .	mm3838			ine	
0 k / 48'390 k in 0 / 132 D	atei(en), 0 / 5 Verzeichnis(se	en)		0 k / 48'390	k in 0 / 132 Datei(en), 0 / 5 \	/erzeichnis(sen)		
acr\Exhibition_Examples\A	AutochemCrysalisProvdhol27	binned>						
F3 Anzeigen	F4 Bearbeiten	F5 Kopieren	F6 Be	rwegen	F7 Neuer Ordner	F8 Löschen /	UI+F4 E	eit:



Uster (flucaliburdata),20110827_juci/Est	ubition Examples Aut	ochemCrysalsPro?	dhoQ7 binned	Aframestahol27	- 0 -
Den Saarbeiten Optonen Coderung Hife OD SAPPHIRE 3.0 COMPRESSION=TY7(22.8)					43
NX: 512 NY: 512 OI: 1067 O NHEADER: 5128 NG: 512 N NSUDPLEMENT: 8	L= 0 S= 768 NK=	1024 NS=	512 NH=	2048	
TIME=Sat Oct 05 15:42:45 201	3	96			87
9600 ž €F8 N9 2.5.0.3	1∕Ie0-ŠĂŕ	Vila			

\$16¤-ÝŤ]e.82Ttq¹2UtAffgag`s´QZ-×ÍfP-i!lTçyÖ´±e]A8X\$7,6+ÓXgeŐőj^L**''²²-gfJ+ş\$uF\$-6+g6+ :LNAFO+__f=vÚ!GĔTsNK)v^{*}ec[[EXKF׍∎f¤,joLQ1ŠN6+jfD/\$-Ja1HA*vîfÚut&fş+*'Ç2]f0+2A/nDT2a ©-1+82Ŭ+U+1[U\$__óyě+ff2*[i]*L]ex]f\$X#6gfŤ

\$UUFR`{DCIDS`*TU^{**}DS`_AQ`'_12f5*tD2KUuy-deeIt'D`UExQuO`_`{CT8:6L5geqF8At`**UEx6Af`s`` 6q`ë9L`u=6/U+Tu`]Dx`_\f6+CU`\$S\$F0:Qe`!DrAqT]!tqf0EL.dx;UrxgFyqba(UIC&Tjf`yh`]IfK*`9F8 L`Utxf1TC&WTD01L``&KFC3KUC`*T28FRU.kE.uX2*qF1R2t)2T]`**UD#u\$:FEW{FN}1A5``{K^iq4F 2-**CI5xy]{g=bdZ`c.WF`6-t>22EF,`UQ=\$U`]PEI)`f:dIEU/53.\Q

gÇi6..eZ'Ly1Îdduô

Ex.FIdixuTMn-AUnpellOndShl_16ytt4Ctt_F+ 2'w8tk(_ig_''|-A'+0LTES=7A.KAF4Z3q'd'4556vU2:]j4\$,u126[]zémEijefN-N, TL'-CUTC95[51:A02'+AF-0a/+10Vµ["e,-L/t'iy ÉqFeéhe(j'|Ift-F0;g] /6F"212[ff",-S-F@Hur269-h5-FL;u,L[5/h26f']A[72]UJXB2F1h652rS':NF]-u MS6Tµ[3]YgSSuut ...FRVTq)×E§642FaG:u[ptL-t6zth05"c2a6"67"_t5F+tELn[6(V6F+S5)Eq]61?]Se b(28F0U1'0g9DUK 1f75µ/sub-as"W ±L+b- InSvie49(FC K Wn g &S-EU;"0'Z5]fz_\$z2UDFt35'd'NN60_L2COF_v & /ig4pdftA5p-19]-2f[(JNR+-cN kgA'T6]za82']L2F409865*TT"F156.56UT"iteX]i:A''c-1 eUE>(Uxµt]T.%260efT\$_tz--AsTmfa6t*WU+OzUc6a=t2q6++c__S4UD%21Fddd9' TLaME*F2i21U' Cs_IF00Z73Ege62ElEheA1vzIRS-16"+18; [&edf1yU+s*]0'ni=SaF4_U"'UASZDUU"'Iv6b]R#gPE _iSK-2dU'vC15IS05918.yuh+tu(w)ZS<zkLfN604gc][egeAdRht±4ZtC+h5o-_Z<<iflivef0)_"'+ -AisECn





Datel Bearbeiten Optionen Codierung Hilfe

(.HEADER BYTES: 4096: BYTE ORDER: little endian: COLLISION INFO:C:/Rigaku/Cr ustalClear/Administrator/LV_XLP/LY20141211-02/Images/Collision.xml:.COMMENT :.COMPRESSION=None:.CRYSTAL_GONIO_COLLISION_OFFSET=0 0 0:.CRYSTAL_GONIO_DE SCRIPTION=AFC12 (Right): Kappa 3 circle: CRYSTAL_GONIO_NAMES=Omega Chi Phi: .CRYSTAL_GONIO_NUM_UALUES*3;.CRYSTAL_GONIO_SCAN_AXES*Omega Phi :.CRYSTAL_GO NIO_SERUER_UERSION=MSCServDetCCD 5.7.4.8;.CRYSTAL_GONIO_UNITS=deg deg deg;. CRYSTAL GONIO VALUES:0.0000 0.0000 18.0000: CRYSTAL GONIO VALUES MAX:205 8 2 360:.CRVSTAL_GONIO_UALUES_MIN=-110 -82 -360:.CRVSTAL_GONIO_UECTORS=1.0000 0.0000 0.0000 0.6428 0.0000 0.7660 1.0000 0.0000 0.0000; DETECTOR_NAMES=P ILT_:.DETECTOR_NUMBER=1:.DETECTOR_TYPE=Pilatus 200K:.DIM=2:.DTDISPLAY_ORIEN TATION=-X+Y:.DTINTEGRATE_OBLIQUE=5 0 -0.06030 0 -0.04670 0 -0.00059 0 -0.02 689 1 -14.88; DTREK_DATE_TIME=12-Dec-2014 01:05:51; DTREK_MODULE=dwTREK; DT REK UERSION=dxTREK version 9.9.9.10 W9RSSI -- Sep 24 2014: Data tupe=long i nt:.FILENAME=LY20141211-02_Cu2356.img:.HEADER_UERSION=1.2:.OBLIQUE_CU=5 0 -0.06030 0 -0.04670 0 -0.00059 0 -0.02689 1 -14.80000:.0BLIQUE_MO:5 0 -0.006 21 0 -0.00603 0 -0.00073 0 -0.00276 1 -1.55000: OPTICS_COLLIMATOR=0.3 x 1.5 Double Pinhole: .OPTICS_TYPE=Confocal: .ORIGINAL_IMAGE_FORMAT=CBF_DTREK: .PIL T_DETECTOR_ADC_OFFSET=0:.PILT_DETECTOR_DESCRIPTION=PILATUS conversion:.PILT DETECTOR DIMENSIONS=487 487: PILT DETECTOR IDENTIFICATION=Dectris Pilatus2 00K_SN02000167: PILT_DETECTOR_OPTIONS=trigger:on: PILT_DETECTOR_SERVER_VERS ION=RigakuMultiServer 1.1.0.13; PILT_DETECTOR_SIZE=83.7640 70.0040; PILT_D ETECTOR_VECTORS=1 0 0 0 1 0: PILT_GONIO_COLLISION_OFFSET=0.0 0 0.0 0.0 0: PILT_GONIO_DESCRIPTION=AFC12 (Right): 2theta arm: PILT_GONIO_NAMES=RotAb outBeam 2Theta Roty XShift YShift Distance: .PILT_GONIO_NUM_UALUES=6: .PILT_G ONIO_UNITS=deg deg deg mm mm mm:.PILT_GONIO_UALUES=0.0000 0.0000 0.0000 0.0 000 0.0000 35.0000; PILT_GONIO_UALUES_MAX=0.0 115 0.0 0.0 0.0 136.56; PILT _GONIO_UALUES_MIN=0.0 -20 0.0 0.0 0.0 30; PILT_GONIO_UECTORS=0.0000 0.0000 1.0000 1.0000 0.0000 0.0000 1.0000 0.0000 1.0000 0.0000 0.0000 0.0000 0 .0000 1.0000 0.0000 0.0000 0.0000 -1.0000: PILT_NONUNF_INF0=FirstScanImag DTI T NONIME TUDE-CINCID BOOK . DTI T CENCOD TUTCYNESS-0 001000. DTI T CEDTO

0.%

🔡 [2] Total Commander 8.0 - NCT REGISTERED									.
Eles Mark Commands Net Show Configura	tion Start								Help
🖉 111 💽 🖬 🖄 🐁 🔶 🤿	1 🏦 🌐	5 8	8 8	85	¥ 🏚 🖉 🗅 🗅				
	RA		1			2,572,000 k free			X.
code SAPPHIRE UNCOMP 300k diamond H	F007 MCCD	frames			Fraser_jump 2013 06 14 Agilent P	oliah Day DataE	Backup protoc	la	
F\Data\2013\Fraser_jump\trames* *			*	•	<pre>sf\Data\2013\Fraser_jump**</pre>				* *
Name	Ext Size		Jate		Name	E	bt Size	+Date	
Calip 1 1	img 271	,744 02	/12/2013	1.	金山		<dir></dir>	07/17/201	13 1 🔺
Sip 1 Z	ing 2/1	.744 02	/12/2013		lexpintol		<dih></dih>	0//02/201	13 1
Usip 1 3	ing 271	744 02	/12/2013	1 = 1	[frames]		DIR>	07/24/201	13 1
Jelip_1_4	Ing 271	,744 02	/12/2013	1			<dir></dir>	07/18/201	13 1
Islip_1_5	ing 271	,744 02	/12/2013	1	[movie]		<dir></dir>	06/12/201	13 1 _
Jalip_1_6	ing 271	,744 02	/12/2013	1	[movie after]		<dir></dir>	06/12/201	13 1
slip_1_7	ing 271	.744 02	/12/2013	1	[movie before]		<dir></dir>	06/12/201	13 1
Jalip_1_8	ing 271	,744 02	/12/2013	1	[New folder]		<dir></dir>	OG/28/201	13 1
Elip_1_9	ing 2/1	,744 02	/12/2013	1	[i][piots_dc]		<dih></dih>	0//15/201	13 1 🛄
elip_1_10	ing 271	,744 02	/12/2013	1	[plote_red]		<dir></dir>	07/15/201	13 1
shp_1_11	inng 271	.744 02	/12/2013	•	[struct]		<dir></dir>	06/12/201	13 1
slip_1_12	ing 271	.744 02	/12/2013	1	[tmp]		<dir></dir>	07/02/201	13 1
slip_1_13	Ing 271	.744 02	/12/2013	1	slip_cracker	pi	ar 18,2	9 07/17/201	13 1
slip_1_14	ing 271	.744 02	/12/2013	1	slip_peakhunt	ta	ibbin 181,3	6 07/17/201	13.1
-Jslip_1_15	ing 271	.744 02	/12/2013	1	slip_selexpinfo_1_G		sl_od 3,9	2 07/17/201	13 1
-Jelip 1 16	imo 2/1	.744 02	/12/2013	1	CrysalisExpSettings	in	1,4	9 0//1//201	13 1
-Jolip_1_1/	ing 2/1	.744 02	/12/2013		alip	ta	abbin 2,74	6 0//1//201	13 1
sip_1_16	ing 2/1	.744 02	/12/2013		sip_red	s	JIN 54,31	13 07/02/201	13 1
-Velip_1_19	ing 27	.744 02	/12/2013	11	elip	a	f_cd 7,2	0 07/02/201	13 1
-Usip_1_20	ing 271	744 02	/12/2013	11	sip	a	I 7,23	0 07/02/201	13 1
L sup_1_71	ing 771	744 07	/12/2012	÷ 1	Parties .		ki :2,64	A 07/02/201	12 1
Ti-li- 1 22	ing 271	744 02	/12/2013	÷ 1	all all a		4- 22	C 07/02/201	13 1
Take 1.24	ing 271	744 02	/12/2013	4 1	sup	0.	40 2.5	0 07/02/201	13 1
Islin 1 25	ima 271	744 02	/12/2013	i I	l slin	, in the second s	dtmn 526	4 07/02/201	13 1
Island 1 25	ima 271	744 02	/12/2013	i 1	alia.		mod 20.9	2 07/02/201	13 1
Isip 1 2/	ima 2/1	/44 02	/12/2013	i I	sio		porot 2/3/2	2 0//02/201	BT
Islip 1 28	ima 271	.744 02	/12/2013	i I	slip profitpeak	ta	bbin 191.1	6 07/02/201	13 1
Islip 1 29	Img 271	744 02	/12/2013	1	slip hid edgeskip	te	t 9	0 07/02/201	13 1
Isip 1 30	ima 271	744 02	/12/2013	1	slip bid skiprenion	te	t 34	2 07/02/201	13 1
Jalip 1 31	imu 271	744 02	/12/2013	1	slip hkl overflow	La La	a	6 07/02/201	13 1
Islip_1_32	ing 271	744 02	/12/2013	1	8. proffitloop	m	ac 3	9 07/02/201	13 1
🧐 slip_1_33	ing 271	,744 02	/12/2013	1	slip_pl_	pr	offitpars 2,0	0 07/02/201	13 1
islip_1_34	ing 2/1	,744 02	/12/2013	1	slip_pijump	p	rottitpars 2,04	0 07/02/201	13 T
Telin 1 25	ima 271	744 02	/10/0013	1 *	Relin of issue overspel: 100		offitnare 20	0 07/02/201	12.1 *
2,388 k / 130,860 k in 9 / 493 file(s), 0 / 3 dir(s)					0 k / 190,087 k in 0 / 128 file(s), 0	/ 11 dir(s)			
f:\Data\2013\Frase	r_jump>								-
F3 View F4 Edit	F5 Cop	y		F6 M	F7 NewFolder	F8 Delete	e	Alt+F4 Ext	

Champe data brain.		121100-002	安美 湯田市			
Page 1	10.47					
Company Spanst - Patron	14.45	1.00	sa . here an entries of the time	a free		1.4
Tan Ashaala	An 100-10	5	Front, Jone - 2022 SC 14, Aglant Fullet, Rep.	fide disting	-	
Common Rev Contents		1 4 4	Infoldation Providence			
Annual Arts		A COMP.	Plane	1.00	100	diam.
And and an other states of the state of the		monate to	167.5		100-	EXTLORED
The state of the second state of the second state.	1252.005	Including to the	Second and		CHIED.	DESIGNATION.
Page Page	40-0161	20/10/0812 10	Barrel		dillo	11/04/04/21
Chang Tranged March	104 A	MANNED IN P	deal		-188.4	61/16/0010
Auto-Deserve Tax 2	Callence of the local division of the local	TRUTINGEN H	_manual		dillo.	86/61/00001
Association and	- China	BACTON DELS 4	Secondary aller		-1968-1	BE/G/OPER
		DOVENUELD IN	line dia linfordi		1000	96/10/0813
		BOV OVORIES N	Officer Autobiot		1000	BLOBORD.
and the		BATMAN S.	There and		1000	\$17370843
		30/10/2013 1	Bern and B		100	EV-EVIDED.
and the second se		BUILDING TO A	CONTRACTS		-010	IN/10/JPCF
Transaction (and a feature fragments		NO WARTS 4	and the second s		-0980	EX-RECORDS
(Development (1988, 198, 106, 106, 106, 106, 106, 106, 106, 106		00/10/019151	Prop CLEAN.		18.2 17	EX-14-DETS
Jonne Graveslei Dilej Affeld, Mill, Mill.		any same sa	our linearest		110,000	E2-11-04-1
Werts Providences Phase mechanisms		BOY SOUTH 1	Mar. padropander, 1, 8	84.34		EV-LOOPER
And the second se		BOY LOVERS 1	Constant accountings		10.42	EV LUGISS
.54	ALM .	Burlaness a	Sec. and		14 1911	and the states of
- 1 H		A STATISTICS IN CONTRACTOR		100	1000	CONCERNING IN
		A REPARTMENT OF	1000	1.0	1000	A A TRACE AND A
and the second sec	102 74	A MUNICIPAL T		- II.	10.000	WINSAME.
	10.14	a hoursheld at a	1.2			California
de 120	301.74	KC/D/DET3.8	1		2.26	KURLOPP.
and 1.28	117.34	NUCLASSIN I		-	4 100	62.62-2019
1.25	717.14	EUCOMMENTS N	-	1000	127.654	ELTER-OMET
No. 1 26	207.24	1 C100/02/02 1	- de	- American -	20,027	AVELORD.
in 107	201.34	KI/GODINT	1.000	mand	101260	EXELUTION IN
49 1 10	101.04	4 donto/det 3 1	de preferante	addate:	101.330	EXTRUDET.
www.1.02	107.4	4.8010/08121	one the observed	- 100	306	EATERSTEEL.
Aug. 1.100	10.34	1.02103-0210-021	the last photospec	144	940	63/63/3643
HALL AL	NO 10 04	4 62/ B/2010 L	Citto 198, realized			63/63/2015
46.1.32	101,34	A REVENUE AND	(Nordeling)	med .	199	KERE-MIN
wig.1.00	30.24	1 20/10/2011 1	Mar. pl.,	and the set	n 2,680	KERELOPES.
No.1.N	111.36	P 2130/10/0811 1	Call (Long)	and they a	n (2.68)	EX/EX/ORX
1. M	TV: 10	A.MUTADATA ST.	Take 11. Inter second CR		1.188	STATISTICS.
889 # 7 \$30.860 # in # 2 839 9860; \$7.74 #80			THE PARTY OF A PARTY PARTY AND A PARTY OF A			

💾 Multi-Rename Tool			
Rename mask: file name	Extension	Search & Replace	Define counter [C]
slip_1_0[C]	▼ [E]	Search <u>f</u> or:	Start at: 1
[N] Name [YMD] [N##] Bange [hms] I [C] Counter [=?] Plu	Date [E] Ext. ime [E##] Range igin [C] Counter	Replace with: □^ □ tx ♥ [E] □ RegEx Su Upper/lowercase Unchanged	bst. 2 F2 Load/save settings ▼
Old name Ext.	New name	Size Date	Location
slip_1_1.img slip_1_2.img slip_1_3.img slip_1_4.img slip_1_5.img slip_1_6.img	slip_1_01.img slip_1_02.img slip_1_03.img slip_1_04.img slip_1_05.img slip_1_06.img	271,744 02/12/2013 12:27:0 271,744 02/12/2013 12:27:1 271,744 02/12/2013 12:27:1 271,744 02/12/2013 12:27:1 271,744 02/12/2013 12:27:2 271,744 02/12/2013 12:27:2	6 F:\Data\2013\Fraser_jump\frames\ 0 F:\Data\2013\Fraser_jump\frames\ 4 F:\Data\2013\Fraser_jump\frames\ 8 F:\Data\2013\Fraser_jump\frames\ 5 F:\Data\2013\Fraser_jump\frames\ 6 F:\Data\2013\Fraser_jump\frames\
slip_1_7.img	slip_1_07.img	271,744 02/12/2013 12:27:2	9 F:\Data\2013\Fraser_jump\frames\
slip_1_8.img slip_1_9.img	slip_1_08.img slip_1_09.img	271,744 02/12/2013 12:27:3 271,744 02/12/2013 12:27:3	3 F:\Data\2013\Fraser_jump\frames\ 7 F:\Data\2013\Fraser_jump\frames\
Please press 'Start!' to start re	naming!	Start! Unde	Result list Close



Import tools

- Easier access to import/export options (on power toolbar).
- 2. Organized export options.
- 3. Importing external images on one clique (instead of typing commands).
- 4. Esperanto importer for non standard image types.





Known formats and esperanto





the second second

Copyright © 2016 - Rigaku Corporation and its Global .

The design attents yes in particle generation of the life and discuss for for the descendence of a DTHD, when an I show a strange for returning Theorem (above a grant for the data DTHD) and for any answer (BEL resp I - Channel and the low much returning the low data for the second strategy of the low second strategy of

External Frame & File Formats

Rigaku – dtrek format







Run list and aliases file generator for DTREK data collections

This dialog allows you to quickly generate a *.run file and aliases file for the data reduction of a DTREK data set!

1. Select an image, by clicking 'Browse' button in group box First dc DTREK dc file, e.g. name1001.img

- 2. Choose whether instrument model will be loaded from selected image header or selected par file
- 3. Terminator format is automatically set, but you can change it if necessary

4. Also the last image will be automatically found, but you can change it if necessary (if it is not automatically found) Note: It is assumed that all frames between these two are available

5. Save the file

- You will be prompted for entering some critical parameters (usually default values are OK, as they are taken from image headers)

- Finally a new CrysAlisPro instance will be launched with the DTREK data set added to the experiment list

NOTE: Using CrysAlisPro you can process only DTREK images from selected Rigaku detectors! R-AXIS format is not supported!

1. First de DTREK de file (*1001.img.)

Browse E:\data\2015\04\Alaska Images_2\MM007Cu\140304_screen0001.img

Image information: detector distance=35.00, wavelength=1.541870, centerx=244.4, centery=206.2, Si thickness=1.000mm

4. Last de DTREK de file

Run TC

Help

Browse E:\data\2015\04\Alaska Images_2\MM007Cu\140304_screen0018.img



x

Example: Apex data from ECM-Basel

- Handling of twin data...
- Dr. Daniel Kratzert (Freiburg, Germany) reduced a Bruker Apex2 twin with CAP and Saint.
- This presentation gives the workflow for importing and reducing Bruker data and handling twinning
- For the evaluation the forum version 38.43 was used.



Data set import



0 k / 763.252 k in 0 / 2895 file(s)



	Known format selector (1.0.1)	
	Known formats with valid headers	
	C Dtrek (Rigaku) rigaku - CCD/Pilatus, no curved IP	
options	C MAR/Rayonix marNNNN, pck, img - IP, CCD, Rayonix with Mar f	ormats
Known image format (with valid image headers)	 Saxi (Bruker) sax, sfrm - smart (with unwarp format), Apex, Photon50/100 	
Transform unknown image format to esperanto	C Dectris cbf - simple setup with single spindle type PX	
	Note: Known formats with unsupported headers may be transformed	
Cancel	to Esperanto format with an Esperanto importer.	nporter

- Open any existing experiment
- Import button

Copyright © 2016 - Rigaku Corporation and its Global .

Data set import

Run list and aliases file generator for SAXI data collections	
This dialog allows you to quickly generate a *.run file and aliases file for the data reduction of a SAXI data set!	
1) You select image name_1_1.sax or name01.001 or name_01_0001.sfm	
2) You select the last image to be considered (It is assumed that all frames between these two are available)	
3) Save the file	
4) You will be prompted for entering some critical parameters (usually default values are OK, as they are taken from image heade	(5)
5) Finally a new CrysAlisPro instance will be launched with the SAXI data set added to the experiment list	
NDTF: Using CrussialisProlycy can process only SaXI images from APEX1 and APEX2 detectors	
First dc SAXI dc file (*_1_1.sax or *01.001 or *_01_0001.sfm)	
Browse E:\data\2016\08\bruker\DK_ML7-66_MM_3843\DK_ML766_01_0001.stm	
	Destile
Last do SAXI do hie	Partile parameters
Browse E:\data\2016\08\bruker\DK_ML7-66_MM_3843\DK_ML766_07_0455.sfm	
	Please enter partile parameters: binning detecto
Help Cancel Save run file	wavelength centery
	2 41 00 0 710730 515 30 510 30
	Provide and a second second second second second second

Open any existing experiment

OK

• Import button



Cancel

Data set facts

- Mo, Iµs, no Si filter showoing 3λ effect
- Frame width: 0.4, correlated ? Frames

CrysAlisPro run list data

a colle	ection mo	de: correla	ated									
al numb	ber of fr	ames:2889	(scan: 28	89, reference	: 0)							
k space	e: 763.79	Mb										
roximat	te data c	ollection [.]	time (h:m	in): 10:55								
t s	start	end	width	exposure	:	speed-rat	omega	theta	kappa	phi	# to do f	# done
0	1.386	184.186	0.400	5.000+	5.000	0.000	-	30.000	73.926	-0.814	456	456
0 -	-11.114	171.686	0.400	3.000+	3.000	0.000	-	17.500	73.926	4.186	456	456
0	21.376	163.775	0.400	3.000+	3.000	0.000	-	10.000	73.926	86.686	356	356
0	21.786	174.186	0.400	3.000+	3.000	0.000	-	20.000	73.926	-35.816	380	380
0 -	-28.114	126.686	0.400	5.000+	5.000	0.000	-	-27.500	73.926	11.685	386	386
0	18.386	179.186	0.400	4.000+	4.000	0.000	-	25.000	73.926	9.184	401	401
0	-7.815	174.186	0.400	3.000+	3.000	0.000	-	20.000	73.926	-60.814	454	454
	a coll al num k spac roxima t o o o o o o o o o o o	a collection mo al number of fr k space: 763.79 roximate data c t start o 1.386 o -11.114 o 21.376 o 21.786 o -28.114 o 18.386 o -7.815	a collection mode: correl al number of frames:2889 k space: 763.79Mb roximate data collection t start end o 1.386 184.186 o -11.114 171.686 o 21.376 163.775 o 21.786 174.186 o -28.114 126.686 o 18.386 179.186 o -7.815 174.186	a collection mode: correlated al number of frames:2889 (scan: 28 k space: 763.79Mb roximate data collection time (h:m t start end width o 1.386 184.186 0.400 o -11.114 171.686 0.400 o 21.376 163.775 0.400 o 21.786 174.186 0.400 o -28.114 126.686 0.400 o 18.386 179.186 0.400 o -7.815 174.186 0.400	a collection mode: correlated al number of frames:2889 (scan: 2889, reference k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure o 1.386 184.186 0.400 5.000+ o -11.114 171.686 0.400 3.000+ o 21.376 163.775 0.400 3.000+ o 21.786 174.186 0.400 3.000+ o -28.114 126.686 0.400 5.000+ o 18.386 179.186 0.400 4.000+ o -7.815 174.186 0.400 3.000+	a collection mode: correlated al number of frames:2889 (scan: 2889, reference: 0) k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure o 1.386 184.186 0.400 5.000+ 5.000 o -11.114 171.686 0.400 3.000+ 3.000 o 21.376 163.775 0.400 3.000+ 3.000 o 21.786 174.186 0.400 3.000+ 3.000 o -28.114 126.686 0.400 5.000+ 5.000 o 18.386 179.186 0.400 4.000+ 4.000 o -7.815 174.186 0.400 3.000+ 3.000	a collection mode: correlated al number of frames:2889 (scan: 2889, reference: 0) k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure speed-rat o 1.386 184.186 0.400 5.000+ 5.000 0.000 o -11.114 171.686 0.400 3.000+ 3.000 0.000 o 21.376 163.775 0.400 3.000+ 3.000 0.000 o 21.786 174.186 0.400 3.000+ 3.000 0.000 o -28.114 126.686 0.400 5.000+ 5.000 0.000 o 18.386 179.186 0.400 4.000+ 4.000 0.000 o -7.815 174.186 0.400 3.000+ 3.000 0.000	a collection mode: correlated al number of frames:2889 (scan: 2889, reference: 0) k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure speed-rat omega o 1.386 184.186 0.400 5.000+ 5.000 0.000 - o -11.114 171.686 0.400 3.000+ 3.000 0.000 - o 21.376 163.775 0.400 3.000+ 3.000 0.000 - o 21.786 174.186 0.400 3.000+ 3.000 0.000 - o -28.114 126.686 0.400 5.000+ 5.000 0.000 - o 18.386 179.186 0.400 4.000+ 4.000 0.000 - o -7.815 174.186 0.400 3.000+ 3.000 0.000 -	a collection mode: correlated al number of frames:2889 (scan: 2889, reference: 0) k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure speed-rat omega theta o 1.386 184.186 0.400 5.000+ 5.000 0.000 - 30.000 o -11.114 171.686 0.400 3.000+ 3.000 0.000 - 17.500 o 21.376 163.775 0.400 3.000+ 3.000 0.000 - 10.000 o 21.786 174.186 0.400 3.000+ 3.000 0.000 - 20.000 o -28.114 126.686 0.400 5.000+ 5.000 0.000 - 27.500 o 18.386 179.186 0.400 4.000+ 4.000 0.000 - 25.000 o -7.815 174.186 0.400 3.000+ 3.000 0.000 - 20.000	a collection mode: correlated al number of frames:2889 (scan: 2889, reference: 0) k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure speed-rat omega theta kappa o 1.386 184.186 0.400 5.000+ 5.000 0.000 - 30.000 73.926 o -11.114 171.686 0.400 3.000+ 3.000 0.000 - 17.500 73.926 o 21.376 163.775 0.400 3.000+ 3.000 0.000 - 10.000 73.926 o 21.786 174.186 0.400 3.000+ 3.000 0.000 - 20.000 73.926 o -28.114 126.686 0.400 5.000+ 5.000 0.00027.500 73.926 o 18.386 179.186 0.400 4.000+ 4.000 0.000 - 25.000 73.926 o -7.815 174.186 0.400 3.000+ 3.000 0.000 - 20.000 73.926	a collection mode: correlated al number of frames:2889 (scan: 2889, reference: 0) k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure speed-rat omega theta kappa phi o 1.386 184.186 0.400 5.000+ 5.000 0.000 - 30.000 73.926 -0.814 o -11.114 171.686 0.400 3.000+ 3.000 0.000 - 17.500 73.926 4.186 o 21.376 163.775 0.400 3.000+ 3.000 0.000 - 10.000 73.926 86.686 o 21.786 174.186 0.400 3.000+ 3.000 0.000 - 20.000 73.926 -35.816 o -28.114 126.686 0.400 5.000+ 5.000 0.000 27.500 73.926 11.685 o 18.386 179.186 0.400 4.000+ 4.000 0.000 - 25.000 73.926 9.184 o -7.815 174.186 0.400 3.000+ 3.000 0.000 - 20.000 73.926 -60.814	a collection mode: correlated al number of frames:2889 (scan: 2889, reference: 0) k space: 763.79Mb roximate data collection time (h:min): 10:55 t start end width exposure speed-rat omega theta kappa phi # to do # o 1.386 184.186 0.400 5.000+ 5.000 0.000 - 30.000 73.926 -0.814 456 o -11.114 171.686 0.400 3.000+ 3.000 0.000 - 17.500 73.926 4.186 456 o 21.376 163.775 0.400 3.000+ 3.000 0.000 - 10.000 73.926 86.686 356 o 21.786 174.186 0.400 3.000+ 3.000 0.000 - 20.000 73.926 -35.816 380 o -28.114 126.686 0.400 5.000+ 5.000 0.00027.500 73.926 11.685 386 o 18.386 179.186 0.400 4.000+ 4.000 0.000 - 25.000 73.926 9.184 401 o -7.815 174.186 0.400 3.000+ 3.000 0.000 - 20.000 73.926 -60.814 454



First opening of the data set

Select SM/PX nature

Name	Path	Created	Accessed	Chemical
mrp160014	E:\data\2016\04\Newcastle Face Indexing\mrp160014_copy	Fri Feb 26 12:07:29 2016	Wed May 25 17:59:06 2016	C6 H8 O6
exp_66	E:\data\2016\04\warrick_movie issue\exp_66_copy	Wed Apr 13 06:32:20 2016	Tue Jun 14 14:10:08 2016	???
w2new	E:\data\2016\04\warrick_movie issue\jw2new_copy	Sun Apr 10 08:13:28 2016	Thu Jun 16 18:40:29 2016	C20 H20 N
xp_48	C:\XcaliburData\Mathias_PX_screens\exp_48	Thu May 19 13:09:32 2016	Mon May 23 08:34:47 2016	???
50716_CudppaO2dppm	E:\data\2016\05\saturn_fixedchi\FixedChi-Saturn	Mon May 30 11:07:06 2016	Mon May 30 11:07:09 2016	???
50716_CudppaO2dppm	E:\data\2016\05\saturn_fixedchi\full	Mon May 30 11:20:22 2016	Mon May 30 11:20:26 2016	C300 H256
Cu_Near48mm	E:\data\2016\05\biberach\calib_XtaLAB_Mon-May-30-18-10-13	Mon May 30 16:11:22 2016	Tue May 31 09:57:45 2016	???
3ICR_L35_260x_2p25_	E:\data\2016\05\20160510_p300k_frx\unpack	Tue Jul 21 11:28:37 2015	Tue May 31 10:43:43 2016	C616 H963
pre_exp_5	E:\data\2016\05\biberach\email1\exp_5	Mon May 30 16:03:24 2016	Tue May 31 11:51:33 2016	???
est	E:\data\2016\05\biberach\Pierre	Tue May 31 08:51:38 2016	Tue May 31 13:33:58 2016	???
est2	E:\data\2016\05\biberach\BI_SecondDataCollection	Tue May 31 10:51:16 2016	Tue May 31 13:51:08 2016	???
lata	E:\data\2016\06\Japan_Bruker_data\data	Fri Dec 18 05:03:58 2015	Fri Jul 15 10:38:45 2016	C27 H39
re_exp_49	C:\XcaliburData\Mathias_PX_screens\exp_49	Thu Jun 16 09:12:03 2016	running	272
pre_exp_50	C:\XcaliburData\Mathias_PX_screens\exp_50	Thu Jun 16 09:16:36 2016	Wed Jul 13 17:59:30 2016	???
pre_exp_51	C:\XcaliburData\Mathias_PX_screens\exp_51	Thu Jun 16 16:06:51 2016	Thu Jun 16 16:06:51 2016	???
pre_exp_52	C:\XcaliburData\Mathias_PX_screens\exp_52	Thu Jun 16 17:49:31 2016	Mon Sep 05 12:48:04 2016	???
BR-co-PHO A-0193-07	E:\data\2016\07\dusek_twin\IBR-co-PHO A-0193-0721_6	Wed Jun 29 19:01:46 2016	Fri Jul 15 16:42:02 2016	C2 H2 N2
Cy_20160713_2_PAF0	E:\data\2016\07\hypix3000\XLM_INmages	Thu Jul 14 14:40:07 2016	Fri Jul 15 17:29:02 2016	C36 H52
/JR1918_cystiene_30	E:\data\2016\08\george_white\MJR1918_cystiene_300_2	Thu Aug 18 14:32:15 2016	Fri Aug 19 17:47:47 2016	C11 H10 N
)K_ML766	E\data\2016\08\bruker\DK_ML7-66_MM_3843	Tue Sep 06 17:23:54 2016	Tue Sep 06 17:23:54 2016	???
1	m			+





Set the beam stop

Apex system sometimes use a user angle for the beam stop



First peak hunting

• Use default





Automatic unit cell finding

• Use default, 66% indexed, in spite of slightly off model



First instrument model refinement

- The header info is not precise. Refine on full data.
- Use default

oxford diffraction



Use EwaldPro to find the twin

• Find next component in wrong peaks





Use EwaldPro to find the twin

• Easy: 180 deg rotation twin





Use EwaldPro to find the twin

• Back to lattice wizard...





• Run the data reduction wizard. Twin reduction auto set...





an 1: Orientation r	astrix for data r	aduction					
UB - matrix: -0.075024 -0.035193 -0.032212 8.14801 (79.43314 (V = 858.78 elected cell (fro 8.1480 rin 1: 8.14786 9. rin 2: 8.14739 9.	-0.018271 0 0.075135 -0 -0.005098 -0 0.00035) 0.000447) m UM rr/UM tbt 9.4341 11.6 43307 11.60462 43240 11.61012	.032708 (.006240 (.052833 (9.43408 (82.77588 (/UM f): .071 79.43 79.4352 82 79.4352 82	0.000004 0.000006 0.000003 0.00058) 0.00332) 31 82.7755 .7719 79.6400 .7876 79.7054	0.000003 0 0.000005 0 0.000002 0 11.60713 (79.62596 (9 79.6260 8 858.53 1 858.98	(200000) (20000) (20000) (20000) (2000 0 (2000)	12) 17) 2	
attice extinctions	(filter Bravais la (P-lattice)	attice extinction	ons) - Incr	mmensurate s Normal data r Single g-vect	tructures eduction or	(HKL) Edit q	m=0
 Don't use filter Use filter for: 			-	Other (reduct	ine list1	Senerate	Load]

By default the whole experiment will evaluated. To modify this

behaviour edit the run list -->

• Accept the run list

Proffit: CrysAlisPro data reduction assistant (1.0.26) X Simultaneous twin data reduction CRYSALIS Step 2: Experiment run list for data reduction Run list: E:\data\2016\08\bruker\DK ML7-66 MM 3843\DK ML766 .sfm -Image dir: E:\data\2016\08\bruker\DK_ML7-66_MM_3843 width exposure omega detector kappa start end # type start end phi 1.39 184.19 0.40 5.00 30.00 73.93 456 1 o -0.81 1, 2 -11.11 171.69 0.40 3.00 -17.50 73.93 4.19 1, 456 21.38 163.78 0.40 3.00 -10.00 73.93 1, 356 2 0 86.69 21.79 174.19 0.40 3.00 -20.00 73.93 -35.82 1, 380 4 0 -28.11 126.69 0.40 5.00 - -27.50 73.93 11.69 1, 386 5 0 18.39 179.19 0.40 4.00 - 25.00 73.93 9.18 1, 401 6 6 0.40 3.00 -20.00 73.93 -60.81 7 0 -7.81 174.19 1, 454

Rigaku oxford diffraction



Edit start num of selected run

Edit end num of selected run

Copyright © 2016 — Rigaku Corporation and its Global .

• Special pars: All default; Limit the data to 0.75Ang (as done in the B



Background: Smart background

	neous twir	i data red	luction	YSALIS
ep 4: Background	l evaluation			
For an acurate e parameters contr	valuation of integrate of this evaluation: Th	ed intensities a goo ne evaluation rang	od background determinati e Re and the repeat freque	on <mark>is essential. Two</mark> ency Fr.
Re = 50	Edit Re	Fr = 50	Edit Fr	
Binning may redu may use 2 or 4 in	ice the memory required as a first of the second seco	irements for the ba sical memory on ye	ackground evaluation. Defa our machine (risk of swappi	ault is 1. You ng)!
Required disk/r	nemory space for ba	educe backgroun ckground evaluati	on: 47.6/6.3 Mb	type (saves memo
Background for	3D integration			
C Average ba	ckground from 3D c	entroid evalutatior	good for stable & low bac	kground,
C Smart back	ground (combination gh background and	of local and aver locally varying fea	age background computati tures, e.g. protein data, slo	on, good for weak wer)
data with hi				

This is the most critical for the data set: It seems that the Apex detector has unstable background, thus introducing a bias on the average background method. Such behavior is also seen with other detectors where CAP uses by default Smart background.



• Automatic outlier rejection: default

	data reduction assis	tant (1.0.26)		
Simulta	aneous twin	ı data reduc	tion	RYSALIS
Step 5: Outlier rej	ection			
CCD data sets us redundant data c	sually contain more that an be used to check for	n the unique data requi or measurement outliers	ed for the structur	e determination. This
-				
The rejection is b	ased on R. Blessing (1	1997), J. Appl. Cryst. and	additional CCD s	pecific criteria.
The rejection is b	ased on R. Blessing (1	997), J. Appl. Cryst. and	l additional CCD s	pecific criteria.
Outlier rejection is b	ased on R. Blessing (1 utlier rejection	(997), J. Appl. Cryst. and	f additional CCD s	pecific criteria.
The rejection is b Outlier rejection Don't use o	ased on R. Blessing (1 utlier rejection	997), J. Appl. Cryst. and	additional CCD s	pecific criteria.
Outlier rejection is b Outlier rejection Ont use o Outlier Use outlier	ased on R. Blessing (1 utlier rejection rejection:	997), J. Appl. Cryst. and	3 additional CCD s	pecific criteria.
The rejection is b Outlier rejection O Don't use o	utlier rejection	997), J. Appl. Cryst. and	d additional CCD s	pecífic criteria.
Outlier rejection is b Outlier rejection O Don't use o Use outlier r	ased on R. Blessing (1 utlier rejection ejection: 8.14801 9.43408	 (997), J. Appl. Cryst. and 11.60713 79.43314 	f additional CCD s	pecífic criteria. 62596
The rejection is b −Outlier rejection ∩ Don't use o 0 Use outlier r 1 aP I	ased on R. Blessing (1 utlier rejection ejection) 8.14801 9.43408 Use Friedel mates as e	997), J. Appl. Cryst. and 11.60713 79.43314 equivalent	f additional CCD s	.62596
The rejection is b Outlier rejection ○ Dont use o • Use outlier 1 aP ⊽	ased on R. Blessing (1 utlier rejection ejection) 8.14801 9.43408 Use Friedel mates as e	997), J. Appl. Cryst. and 11.60713 79.43314 squivalent	4 additional CCD s	.62596
Outlier rejection is b Outlier rejection O Don't use o Use outlier 1 aP	ased on R. Blessing (1 utlier rejection ejection: 8.14801 9.43408 Use Friedel mates as e	997), J. Appl. Cryst. and 11.60713 79.43314 squivalent	f additional CCD s	.62596



Chem. formula imported for AutoChem

Proffit: CrysAlisPro data reduction assistant (1.0.26)	
Simultaneous twin data reduction	Mu-calculator (1.0.4): Absorption coefficient in mm-1 Cell and wavelength 8.14801 9.43409 Mo-radiation
Step 6: Output	Z: 1.000
Tip: You may change the output name and directory to keep results of data reductions under different parameter sets (UB, supercells) Output file name: E:\data\2016\08\bruker\DK_ML7-66_MM_3843\DK_ML766	Chemical formula: (e.g. C11 H10 S 02); consult help for syntax and special elements (0s) Numbers follow elements; separate elements by space; Import C46 H42 N2 02
Change output name	Result 4 element(s): H= 42.00(6.48); C= 46.00(84.36); N= 2.00(4.28);
Image: Space group determination Image: Automatic Image: Manual Image: Automatic structure solution (AutoChem) AutoChem options C46 H42 N2 O2 Z = 1.00	G= 2.00(4.89); Formula wt: 654.90 Mu(mm-1): 0.08 Density: 1.266 Z: 1.00 F(000): 398.00 At.vol 9.33 Non-H at. vol 17.18
Completeness computation Make unwarp pictures Max order (one for h, k, l): Resolution: 0.80	mu (mm-1) 0.07708 🗖 Edit mu
	Help Set mu and formula Cancel
< <u>Back Next</u> > Finish Cancel Help	



Automatic result

• Auto: based on all hklf4 data.





Tuning your result

• Tuning means what kind of scaling is used and what reflection classes are in the final hklf4 and 5 files

Endetal/20	16109/bioles/04_ML2-66_MM_38	700_9991.080 43
Summetry settings		
12 Use Friedel mates at	equivalent even for noncentrosymm	enic SG
LS refinement control		
SigCut IL		
Exchade III	strongest unique reflections (along	p with all spreadtic expandents)
Frame scaling		8-lactor//k-facilor refinemen
Automatic frame scale	assignment 🗵 Apply Name scale	g T Reline Bractore
How many transes have a common scale?	2 travies = 1 scale •	Refine Arfactori
Variation nutriant (ESD)	0.20000	Tillianes = 7 factor
P Reject frame scales:	[0.20 & x [5:00	Rettaint 0.2000
Empirical absorption correct	on	
Automatic parameter te	dection for absorption correction	
Max even order B	Max add order: 7	+ 80 parameters
Absorption currection b	etine have scaling (recommended	lix shong absorbers!
Delector area scaling		
How many detector area regions?	tet - 1	Apply detector correction
Variation restrant (ESD)	0.20005	



Twin data finalization		CRYSALIS
porof Ries for two finalization DR_ML765.mptwon Septement #1 DR_ML766_twort.mpprof alf 8.543 9.430 properent #2 DR_ML766_twort.mpprof alf 8.544 9.425 Two: finalization log Re (from previous run):	11.603 79.46 82.79 78.63 11.609 79.41 82.80 76.71 DK.JM.Invelog (View 90)	Chensol formula Crist H/2 N2 C2 2 - 1.00 Edit formula Lattue contractly User Trades an estimates an estimates an estimates an
Versions Twin acceptosition Overlap threshold for scaling & space-group determination (0.40) (10) threads Device and completeness in H02-4 (iii) (for struct solution); as one (100 comp	nciel alopack scaling, uniformity, empr	cal absorption Connon scales for all two congenents Generate scales for all two congenents
Numeric and spherical absorption carrection		
Numeric and spherical absorption correction Apple absorption correction Decomprises and structure Secomprises and structure Final Space grass determination Final Space grass determination Final Space Spac	Piters and lattice estinction Alters Recolution No Ster Use filters	C ANY Connection over and the second
Numeric and splemical discreption correction Apply absorption correction Distribution	Pitters and lattice estinction filters Recolution No Ster No Ster No Ster No Cover filters Hit. Se options Pitter of the reflection from component 1 Pitter of the reflection from component	Audy Audy Management the two sets Management Management
HKLF4 result



oxford diffraction

HKLF5 result





Generic image format 'Esperanto' generator

- Use of Esperanto format for unknown image formats with no compression or known formats with strange instrument configs
- Esperanto fully supports 4 circle instruments.
- Command 'dc rit' rit = raw image transform.
- But it also supports the known formats to handle 'unusual', obstinate images.
- Pixel detectors have an automatic dead zone detection based on the special value -1.
- The Esperanto generator uses a proprietary Agilent bit field format. To get back the uncompressed Esperanto version, please use the export function.



Esperanto with bit field compression and pixel detector support

- For our Esperanto importer we now can use Agilent bitfield compression for Esperanto files. The format is not documented yet.
- There was also a pixel detector flag added to support the implemented pixel detector corrections ([dsithicknessmmforpixeldetector] - thickness of Si for pixel detectors; the presence of this number signals a pixel detector. Pixel detector gap zones are marked with -1).
- Publication describes the Esperanto format

Single-crystal diffraction at the Extreme Conditions beamline P02.2: procedure for collecting and analyzing high-pressure single-crystal data

André Rothkirch, G. Diego Gatta, Mathias Meyer, Sébastien Merkel, Marco Merlini and Hanns-Peter Liermann

J. Synchrotron Rad. (2013). 20, 711-720



Dc rit: ADSC 315

out format			
C Known Promiliellen from	+		
and the present of the second	• · · · · ·		
 Generic uncompressed in 	18ge		
Skp header bytest 20	24 x# 3072 y#	3072 Pixel type UNSI	G SHORT (2 BYTES)
Frames info			
Run digitai 📼 👘	Separator Home	France 3 💌 r	emeter ing
F:\Data\2013\inport_e	speranto\ADSC_Quantum_315/	\12mx2jp03_1_001.ing	Browse
PriData (2013) mport_s	speranto (ADSC_Quantum_315r	\12mx2p03_1_005.mg	Browse
		Support data from he	Iders Run TC
seranto output Toranes have name:	adec210 test	Dec It	
nonges voos name.	Increase and	Post +	
Rotation [deg]: 0	C 90 C 180	• 270 T Mirror	
Detector Info			
Detector info Pixel size [mm]: 0.102		1024.0	0 averflavi
Detector info Pixel size [mm]: 0.102 Instrument info	s0= 1024.0 y0w	1024.0	0 averflow
Detector info Ptxel state [rmm]: 0.100 Instrument info Wavelengtho MO	x0= 1024.0 y0+	[1024.0 □ > [59990	0 averflow
Detector info Privel size [mm]: 0.102 Instrument info Wavelength: MO Monochromator:	x0= 1024.0 y0+	1024.0	averfine otran (2010)
Detector info Pixel size [mm]: 0.102 Instrument info Wavelength: MO Monochromator: Alaba: Bate Stach	x0= 1024.0 y0+	1024.0	0 averflaw atran Edit Contactor Edit d-value
Detector info Pixel size [mm]: 0.102 Instrument info Wavelengths MO Monochromator: Alpha, Beta [deg]:	x0= 1024.0 y0x	1024.0 □ > 5000 00000000000 □ Synchr 000000000000000000000000000000000000	averfine atron Edit division
Detector info Pixel size [mm]: 0.102 Instrument info Wavelength: MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kap	x0= 1024.0 y0+ • 0.71, 0.71, 0.63 GRAHITEES 50.0, 0.0 940 [596g]: 0.0, 0.0, 0.0	1024.0 T > 5999 251.415 C T Syndy 251.415 C Syndy 261.415 C Syndy 261.	.0 overfine otron Continuent Edit develoe
Detector info Pixel size [mm]: 0.102 Instrument info Wavelength: MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kapl Detector dist. [mm]:	x0= 1024.0 y0+ ■ 0.71, 0.71, 0.63 GRAPHITE E II 50.0, 0.0 90.0 [Shg]: 0.0, 0.0, 0.0 90.0 [Edit]	1024.0 • 50000 COLORE • 6 9000 COLORE • 6 90000 Colore Edit Bean b2: 0.000 Edit	.0 overfine otron Configuration Edit develop
Detector info Pixel size [mm]: 0.102 Instrument info Wavelength: MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kapl Detector dist. [mm]: Gainu	x0= 1024.0 y0+ ▼ 0.71, 0.71, 0.63 GRAPHITE E IS 50.0, 0.0 90.0 [Sing]: 0.0, 0.0, 0.0 90.0 [Edit 15.0 [Edit]	1024.0	0 overfine otron Conference Fold division et.
Detector info Pixel size [mm]: 0.102 Instrument info Wavelength: MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kapt Detector dist. [tm]: Gain: Scan info IV	x0= 1024.0 y0+ ▼ 0.71, 0.71, 0.63 GRAPHITE E IS 50.0, 0.0 90.0 [Seg]: 0.0, 0.0, 0.0 90.0 [Edit 15.0 Edit	1024.0	0 overfine otron Contractor Fold division
Detector info Pixel size [mm]: 0.102 Instrument info Wavelength: MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kapt Detector dist. [tim]: Gainy Scan info [2] Scan hype:	x0= 1024.0 y0+ 0.71,0.71,0.63 GRAHITEES S0.0,0.0 90.0 Edit 15.0 Edit 9N 0.0	1024.0	0 overfine otron Contractor Fold division et.
Detector info Pixel size [mm]: 0.102 Instrument info Wavelength MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kapt Detector dist. [mm]: Gain: Scan info [2] Scan start, step, expt	x0= 1024.0 y0+ x0= 1024.0 y0+ x0= 0.71, 0.71, 0.83 GRAPHITE E II 50.0, 0.0 90.0 Edit 15.0 Edit 15.0 Edit 0.0, 1.0 Edit	1024.0 > 50000 SPLANE Synchr SPLANE divalue: 3.354 Edit Edit Beam b2: 0.000 Edit Provel d Provel d Omega Free 0.000	0 overfine otron Contractor Fold division et. 0.0
Detector info Pixel size [mm]: 0.100 Distrument info Wavelength MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kap Detector dst. [mm]: Gain: Scan info [2] Scan info [2] Scan type: Scan: start, step, exp: Use frames in inverse	x0= 1024.0 y0x . 0.71, 0.71, 0.83 GRAPHITE E I 50.0, 0.0 90.0 Edit 15.0 Edit 0.0, 1.0, 1.0 Esit order I=last, 2=last-1	1024.0 > 5000 COULDEN Synchr CANE ▼ divalue: 3.354 Edit Beam b2: 0.000 Edit Pavel d Consign Place 0 Theta× 0.0 Consign Place 0	0 overfine otron Contractor Edit devote et. Contractor Kapper 0.0 L000 Edit
Detector info Pixel size [mm]: 0.302 Instrument info Wavelengthi MO Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kapi Detector dist. [mm]: Gain: Scan info IP Scan info IP Scan start, step, exp: Lise frames in inverse	x0= 1024.0 y0x . 0.71, 0.71, 0.83 GRAPHITE E I S0.0, 0.0 90.0 Edit 15.0 Edit 99.0 Edit 0.0, 1.0, 1.0 Esit order 1=lost, 2=lost-1	1024.0 > 50000 COLUCION C Synchr CRANE ▼ dvake: 3.354 Edit Beam b2: 0.000 Edit Provel d Comega Rex 0 Theta× 0.0 C Scan scale er	0 overfine otron Contraction Edit d-value et. Contraction Kapper 0.0 L.000 Edit
Detector info Pixel size (mm): 0.302 Instrument info Wavelengths (mc) Monochromator: Alpha, Beta [deg]: Omega0,Theta0, Kapt Detector dist. (mm): Gain: Scan info (2) Scan info (2) Scan start, step, exp: Cuse frames in inverse Load (2)	x0= 1024.0 y0x 0.71, 0.71, 0.63 GRAPHITE E I S0.0, 0.0 90.0 Edit 15.0 Edit 15.0 Edit 0.0, 1.0, 1.0 Esi order 1=lest, 2=lest-1	1024.0 > 50000 CONTRACT OF Synchr CONTRACT Of Value: 3.354 Edit Beam b2: 0.000 Edit Provel d Conega Rtsc 0 Theta≈ 0.0 Conega Rtsc 0 Conega Rtsc 0	0 overfine otron Edit d-value Edit d-value et. Contraction Kapper 0.0 L000 Edit

- Command dc rit
 - Header bytes 1024, x 3072 y 3072 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
 - Slight play in EwaldPro to get the center right.



Dc rit: ADSC 210

C Known Crystelletro Press			
C	t		
Genenc uncompressed in	uge		
Skip header bytes: 302	2048 yw	2048 Powel type JUNSIG SHORT (2)	BYTES)
Frames info	0 (<u>)</u>		
Run digits 🔝 0	Separator Nome	Frame 3 _ name###.mg	
F:\Data\2013\mport_e	speranto\ADSC_Quantum_210r\1	2mx1jp05_1_001.img	
F: Data 2013 import_e	speranto/ADSC_Quantum_210r\1	2mx1jp05_1_005.ing	
		Import data from headers	Run TC
peranto output			
Images base name:	adsc210_test	Run # 1	
Rutation (deg): 🔿 0	C 90 C 180 G	270 T Mirror	
Detector info			
Pixel size [mm]: 0.102	x0= 1024.0 y0+	1024.0	D/A
Instrument info			
Wavelength: MO	• 0.71, 0.71, 0.63	TOTAL Synchrotron	Liemtete
Monochromator:	GRAPHITE E 1E3	PLANE 💌 divakie: 3.354	(d-value)
Alpha, Beta [deg]:	50.0, 0.0	Edit	
Omega0, Theta0, Kapp	asG [deg]: 0.0, 0.0, 0.0	Edit	
Detector dist. [mm]:	72.0 Edit	Beam b2: 0.000	
Gain:	15.0 Ltdr	T Pixel det.	dit/the
Scan info 🔽			
Scan Type:	C Phy	Gonega Phi= 0.0	
Scan: start, step, exp:	0.0, 1.0, 1.0	Theta = 0.0 Kappa = 0	.0
Use frames in inverse	order 14last, 24last-1	Scan scale er 1.000	EGT
	ie		
Load			



- Header bytes 1024, x 2048 y 20482 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.



Dc rit: MAR165ccd

o importer (1.0.2)		
It format		
Known CrysAlisPro format	MAR marNNNN, pck, img	
Generic uncompressed image		
Skip header bytes: 0	x= 2048 y= 2048 Pixel type UNSIG SHORT (2 BYTES)	-
rames info		
Run digits 💌 0 Separa	ator None Frame 3 nameFFF.img	
F:\Data\2013\import_esperant	to\MarCCD165\data_01_001.mccd Browse	
F:\Data\2013\import_esperant	to\MarCCD165\data_01_010.mccd	
	Import data from headers	
eranto output		
nages base name: da	ta_01_ Run # 1	
otation [deg]: C 0 C	90 🔍 180 C 270 🥅 Mirror	
etector info		
Pixel size [mm]: 0.079	x0= 1035.0 y0= 1031.0 > 99999.0 overflow	
nstrument info		
Wavelength: CU 💌	1.54, 1.54, 1.39 Edit al1, al2, b Synchrotron Edit lambda	
Monochromator:	GRAPHITE E 1E3PLANE 💌 d-value: 3.354 Edit d-value	
Alpha, Beta [deg]:	50.0, 0.0 Edit	
Omega0,Theta0, Kappa0 [deg	g]: 0.0, 0.0, 0.0 Edit	
Detector dist. [mm]: 90.	0 Edit Beam b2: 0.000 Edit	
Gain: 1.0	Edit Edit thk	
Gain: 1.0	Edit Pixel det. Edit thk	
Gain: 1.0 can info Scan type: O P	hi Omega= 57.0 Omega Phi= 75.0	
Gain: 1.0 can info Scan type: O P Scan: start, step, exp: 75.0, 1	Edit Pixel det. Edit thk hi Omega= 57.0 O omega Phi= 75.0 .0, 20.0 Edit Theta= 0.0 Kappa= -134.0	
Gain: 1.0 can info	Edit Pixel det. Edit thk hi Omega= 57.0 Omega Phi= 75.0 .0, 20,0 Edit Theta= 0.0 Kappa= -134.0 elast, 2=last-1 Scan scale err 1.000 Edit	
Gain: 1.0 can info	Edit Pixel det. Edit thk hi Omega= 57.0 Omega Phi= 75.0 .0, 20.0 Edit Theta= 0.0 Kappa= -134.0 =last, 2=last-1 Scan scale err 1.000 Edit)
Gain: 1.0 can info Scan type:	Edit Pixel det. Edit thk hi Omega 57.0 Omega Phi= 75.0 .0, 20.0 Edit Theta= 0.0 Kappa= -134.0 =last, 2=last-1 Scan scale err 1.000 Edit	
Gain: 1.0 can info Scan type:	Edit Pixel det. Edit thk hi Omega= 57.0 Omega Phi= 75.0 .0, 20:0 Edit Theta= 0.0 Kappa= -134.0 =last, 2=last-1 Scan scale err 1.000 Edit	

fraction

- Command dc rit
- Known format MAR (mccd)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

Dc rit: A200 detector

out format C Known CrysAlisPro format			
C Known CrysAlisPro formet			
	· .	*	
· Generic uncompressed ima	Q6		
Skp header bytes: 3584	x# 2048 y#	2048 Pixel type UNSIG SHORT (2 BYTES)
Frames info			
Run digita 🖃 💿 d	Separator Itorie +	Frame 3 • nameFFF.m	0
F:/Data\2013lancert.est	wanto\A206\data2_0201.imit	Drow	
PriData (2013) moort_est	eranto (A200) data2_0220.ing	Brow	10
		Import data trom headers	Run 1C
peranto output			
Images base name:	a200_test	Run # 1	
Rotation Ideal: C o	C 90 (* 100) (270 E Marce	
	The second s	Contra (Contra)	
Detector info	in land	1024.0	11. C
surface and fumit: 10.100	ADE DOZA,O YON	112 CO 1 13 Januaro 100	Turve
Instrument info		and a second	
Wavelengths CU	• 1.54, 1.54, 1,39	Synchrotron 1	st lamdsda
Monochromator:	GRAPHITE E 1E	PLANE 🔹 divakue: 3.354 🛛 🚺	kird-value
Alpha, Beta [deg]:	50.0, 0,0	tar	
Omege0, Theta0, Kappe	0 [deg]: 0.0, 0.0, 0.0	Edit	
Detector dist. [rnn]:	90.0 Edit	Beam b2: 0.000 Edit	
Geint	15.0 Edit	T Pixel det.	Entranc
Scan info 🖓			
Scan type:	🐨 Phi Omega= 0.0	C Omega	
Scent start, step, expt 0	0. 1.0. 1.0	Theta= 0.0 Kappa=	0.0
Lise frames in inverse of	der Inlast, Zulast-1	Scan scale err 1,000	Edit
	11.		3
Load Sove			

- Command dc rit
- Header bytes 3584, x 2048 y 20482 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.



Dc rit: Diamond ID 19 Dectris turned

Known Crysklefthe format DECTRIS Immeric uncompressed amage Immeric uncompressed amage Immeric uncompressed amage Immeric uncompressed amage Immeric I Separator Inderscore • Prame 5 • manuff, FFFFF.img Diddet(2013)(30(3)(0)(dexid pinel(af), scend)/ANAAD_S1deg_1, S80001, ddf Diddet(2013)(30(3)(dexid pinel(af), scend)/ANAAD_S1deg_1, S80001, ddf Diddet(2013)(30(3)(dexid pinel(af), scend)/ANAAD_S1deg_1, S80001, ddf Diddet(2013)(30(3)(dexid pinel(af), scend)/AAAD_S1deg_1, S80001, ddf Pression and PAHAD_S1deg_1, But # Immeric PAHAD_S1deg_1, But # Immer	# format		
Anoun Cryskiphe torme Let Nus	a iornas	a Incorner in	1
Generic uncompressed image Rames info Run digita 1 Separator Inderscore Prame S name#C_FFFFF img D:/dots/2013/10/300k_david_tmal/ad_score/PAHAD_01deg_1_00001.dt/ Inrovae Inrovae Inrovae D:/dots/2013/10/300k_david_tmal/ad_score/PAHAD_01deg_7_00499.ct/ Inrovae Inrovae Inrovae D:/dots/2013/10/300k_david_tmal/ad_score/PAHAD_01deg_7_00499.ct/ Inrovae Inrovae Inrovae D:/dots/2013/10/300k_david_tmal/ad_score/PAHAD_01deg_7_00499.ct/ Inrovae Inrovae Inrovae rearts odput mages base name: PAHAD_01dag_ Run + Inrovae tabletor info 80 188 278 Mercor rearts odput 90 90.0 645 90 Monochriomator: 1.0	 Mnown CrysAldPro forms 	at Joechado -	
Non-odd to the second (PAHAD_SLORg_1_SOUDLAD) Non-odd to the second (PAHAD_SLORg_1_SOUDLAD) Non-odd (PAHAD_SLORg_1_SOUDLAD) Didota/2013/10/3808, david_thref/e8, sciend/PAHAD_SLORg_7_SOUPP.cbl Non-odd (PAHAD_SLORg_7_SOUPP.cbl) Non-odd (PAHAD_SLORg_7_SOUPP.cbl) Non-odd (PAHAD_SLORg_7_SOUPP.cbl) Non-odd (PAHAD_SLORg_7_SOUPP.cbl) Non-odd (PAHAD_SLORg_7_SOUPP.cbl) Non-odd (PAHAD_SLORg_7_SOUPP.cbl) Non-odd (PAHAD_SLORg,7_SOUPP.cbl) Non-odd (P	Generic uncompressed in	nage	
Frances info Run digits 1 Separator Enderscore Prance > name#_FFFFFJing Diddots/2015/10/300k_devid_trief/e8_score/PAHAD_01.deog_1.00001.dt/ Invoice Invoice Diddots/2013/10/300k_devid_trief/e8_score/PAHAD_01.deog_7_00499.dt/ Invoice erents odput Invoice Invoice mages base name: PAHAD_01.deog_ Run + Invoice etestion (deg): 0 180 270 Mcroor Petector info Invoice Invoice overflow notation (deg): 0 180 270 Mcroor Petector info Invoice Invoice overflow Nonochromation: MSR00X/SYNCHROTRON_ Polified: 0.598 Invoice Monochromation: MSR00X/SYNCHROTRON_ Polified: 0.598 Invoice Defector dei: Inmit 1.0 Inter Inter invoice Game 0.00 645 Inter invoice Inter invoice Monochromation: 1.0 Inter Inter invoice Inter invoice Internet 1.0 Inter Inter invoice Inter	Harrison 1	487 6	NA TRUNC - PART -
Bun digits I Seperator Inderscore Prane Pr	Frames info		
Disksin (2013) 10(300)k, dewid_tinel/LeR_scared/PAHAD_01.00g_1_00001.ct/ Disksin (2013) 10(300)k, dewid_tinel/LeR_scared/PAHAD_01.00g_7_00499.ct/ Interest output moges base name: PAHAD_01.00g_ Bun # 270 Microw betector who Pixel size (mm): 0.172 x0 = 300.6 y0 = 323.6 + 10000.0 overflow noticement who Moreochromater: MORROR/SYNCHROTRON(Run digita 💌 1	Separator Underscore 📜 💌 Fra	ime S 💌 nameR_FFFFF.img
D'idete (2013) 2013001, devid, triadial, scares (PAHAD_B1deg_7_00499, cb) erents output mages base name: PAHAD_B138g	Dridetal/2013/10/300k	devid trielleR scens/PAHAD 01deg ;	1-00001.ddf
eranto output mages base name: PHHAD_010Ag_ Run # E sotation (deg): 0 00 190 0 270 Mercor betector srip Peel size (mm): 0.172 x0 = 308.6 y0 = 323.6 P 100000.0 overflow notrument srip Wavelength: IDER V Monochromator: MOREOR/SYNCHROTEDMY Paylect: 0.599 D00 pellos Alpha, Bete (deg): 50.0, 0.0 00 000 Detector des: (mm): 108.0 000 000 000 Detector des: (mm): 108.0 000 000 000 Gam: 1.0 100 000 000 000 Came state Came state Monochromator: 0.000 000 000 Detector des: (mm): 108.0 000 000 Detector des: (mm): 108.0 000 000 Came state Came state	D:\deta\2013\10\3004	devid_trial/al_scars/PAHAD_01deg_1	7_00499.cbf 0iowse
eranto odput images base name: PAHAD_BLAGE, Run # 1 solution (deg): 0 00 180 • 270 Micror Detector site Poel size (mm): 0.172 x0 = 308.4 y0 = 223.8 + 10000.0 overflow natrument site Woreelength: INTER - Monochromator: MISRIOR/SYNCHROTRION Polified: 0.999 000 police Alpha, Bete (deg): 90.0, 0.0 00 000 Detector det. (mm): 108.9 000 000 000 Detector det. (mm): 108.9 000 000 000 Gene: 1.6 Tate Scan state 			Import data from headers Rev TC
eranti olqui images base name: PAHAD_01269_ But # 2 botation [deg]: 0 90 198 # 220 Micror Detector Hfo Pixel size (mm): 0.122 x0= 308.6 y0= 323.6 > 100001.0 overflow natrument Hfo Wavelength: USER * Synchrotition Carl Looks Monochromator: MISROR/SYNCHROTRON(* Polifect: 0.998 Duit realize Alpha, Bete [deg]: 90.0, 0.0 EM Detector det. [mm]: 108.0 ELLIS Beam 0.000 Edit Gen: 1.0 ELLIS Beam 0.000 Edit Stam mfo 90.0 /F Stam solie er 8.020 ELLIS Stam mfo			
Apter des raine: prese cong. and prese cong.	eranto output	Patrian Panas	But #
batetion (deg): 0 180 4270 Mercar betector site Poel size (mm): 0.172 x0 = 308.4 y0 = 223.0 > 100001.0 overflaw habitument sife Image: site in the site in	mayes dese name:	in the second se	Maria 1.
belector sins Poel size [mm]: 0.172 x0 = 308.4 y0 = 223.0 → 100001.0 overflow Instrument sife Wavelength: 10000 → 1000 MOREOR/SYNICHROTRON ♥ Synchrotran for bonds Manachromater: MSROR/SYNICHROTRON ♥ Polliset: 0.998 1000 moles Alpha, Beta [deg]: 90.0, 0.0 104 Detector det. [mm]: 100.0 104 Beam 0.000 dat Beam	Rotation [deg]: 🗇 🛙	○ 90 ○ 180 ● 220	Micror
Pixel size (mm); 0.172 x0 = 308.6 y0 = 223.6 > 0000010 overflaw intrament info Waveleorgth: Intrament info Intrament info Intrament info Intrament info Monochromator: MORROR/SYNCHROTEOM V Synchrotran Intrament info Monochromator: MORROR/SYNCHROTEOM Paylet: 0.990 Dot public Alpha, Beta [deg]: 50.0, 0.0 Iddit Dot public Iddit Detector det: (mm); 100.0 Iddit Iddit Iddit Gam: 1.0 Iddit Beam 0.000 Iddit Gam: 1.0 Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Iddit Idd	Detector info		
natrument info Wavelength: □000	Pixel sze [mm]: 0.172	x0= 308.0 y0= 323.0	o F > 10000.0 overflow
Wavelength: Image: I	instrument atfo		
Monochrumater: MORROR/SYNCHROTRON Poliect: 0.990 Alpha, Beta [deg]: 36.0, 0.0 Col: Dmisga0,Thetad, Kappa0 [deg]: 90.0, 0.0, 0.0 East Detector des. [mm]: 100.0 Col: Cam: 1.0 Col: Cam: 1.0 Col: Cam: 1.0 Col: Cam: 1.0 Col: Cam: Cam: Cam: Cam: Cam: Cam: Cam: Cam	Wavelength: USER	U	Synchrotron I tan lambo
Alphe, Beta [deg]: 98.0, 0.0 (dt Omega0,Theta0, Kappa0 [deg]: 98.0, 0.0 Eu Detector dist. [mm]: 108.0 Cutx Beam 0.000 rds Gam: 1.0 Tutz Praci det. East min Scan mfg 98.0 /7 128.0 200 23.0 00.0 V Scan scale er 8.070 Cut	CONTRACTOR RECORDER	MIRROR/SYNCHROTE	
Append Veter (seg): Sectors Omega0, Thetad, Kappa0 (deg): 90.0, 0.0, 0.0 800 Detector det. (mm): 100.0 600 600 Genn: 1.0 100 600.0 70 100.0 Scan mfg 90.0 /0 100.0 00.0 600.0 Covel Scan scale err 8.070 600.0 600.0	Monochromatori		RDN - Polfact: 0.990 D01polfac
Omigan, Thetall, Kappon (deg): 94.04, 94.04 Deam 0.000 Fda Detector dest. (mm): 108.0 Luix Deam 0.000 Fda Gam: 1.0 Edat Pixel det. Edat min Scan mfg	Monochrometer:	30.0.0.0	ROM Polfect: 0.996
Detector des. (mm): 108.0 Lux Deam 0.000 Lux Gam: 1.0 List IP Pixel det. List with Scan: eff(IP IP IP IP IP Care: IP IP IP IP IP Scan: eff(IP IP IP IP IP Cont IP IP IP IP IP IP Cont IP IP <td< td=""><td>Monochrometer: Alpha, Deta [deg]:</td><td>30.0, 0.0</td><td>RON V Polificiti: 0.990 Fold polifica</td></td<>	Monochrometer: Alpha, Deta [deg]:	30.0, 0.0	RON V Polificiti: 0.990 Fold polifica
Cent: 1.0 tim Poseidet. Edites.	Monochromator: Alpha, Beta [dag]: Omega0,Thetall, Kapp	90.0, 0.0 100 [deg]: 90.0, 0.0, 0.0	ION Polificit: 0.590 EDD polifici
Scan mig 	Monochromater: Alpha, Bete [deg]: Omega0,Thetad, Kapp Detector dist. [mm]:	30.0, 0.0 20 [deg]: 90.0, 0.0, 5.0 108.0 tub	nov police: 0.999 Extraction
00.0 /r 120.0 23.0 23.0 (00.0 ✓ Scan scole err 0.070 Court	Monochromator: Alpha, Deta [deg]: Omega0,Theta0, Kapp Detector dist. [mm]: Gam:	90.0, 0.0 100.0 (deg): 90.0, 0.0, 0.0 100.0 tax Dea 1.0 tax	nov v Polifect: 0.599 EDD pelite fdt tun tun tun tun tun tun tun tun tun tu
25.0 00.0 ✓ Scan scale err 8.070 com	Monochromator: Alpha, Dete [deg]: Omegad,Thetad, Kapp Detector det. [mm]: Gam: Stam mfg	90.0, 0.0 100.0 [deg]: 90.0, 0.0, 0.0 100.0 [deg 1.0 [deg 1.0 [deg	nov v Polifect: 0.999 E.00 pelitect f.dt E.00 E.00 F.dt F.dt F.dt F.dt F.dt F.dt F.dt F.dt
Low!	Monochromator: Alpba, Deta [deg]: Omega0,Theta0, Kapp Detector det. [mm]: Gam: Scam mfg	90.0, 0.0 100 (deg): 90.0, 0.0, 0.0 100.0 100.0 1.0 100.0	ION ▼ Polifect: 0.990 ED0 pelles (dt Euri Euri Pinel det. Euri min (F Pinel det. Euri min (S
Cont See	Monochromator: Alpba, Deta [deg]: Omega0,Theta0, Kapp Detactor dat. [mm]: Gam: Scan. mfg	90.0, 0.0 100 (deg): 90.0, 0.0, 0.0 100.0 100 1.0 100 1.0 100	101 pelles (dt tur tur 0.000 filti (₹ Pixel det turt min 17 - 221,0 100 100,00
Low Seve	Monochromator: Alpha, Dete [deg]: Omega0,Theta0, Kapp Detector dist. [mm]: Gam: Scan.mfu	30.0; 0.0 100 (deg): 90.0; 0.0; 0.0 1.0 1.0 1.0	101 € Polifect: 0.990 E.001 pelles Tolt
	Monochromator Alpha, Dete [deg]: Omega0,Thetath, Kapp Detector dat. [mm]: Gam: Scan mfu	50.0; 0.0 100 (deg): 90.0, 0,0, 0.0 100.0 1.0 1.0 1.0 1.0	101 € Polfect: 0.999 E01 pelke Colt Colt Euro Euro F Pisal det. Ent MA (7 Fisal det. Ent MA (7 Fisal det. Ent MA (7 Fisal det. Ent MA (8,870 Colt
	Monochromator: Alpha, Dete [deg]: Omega0,Thetath, Kapp Detector dat. [mm]: Gam: Scan mfg	50.0; 0.0 100 (deg): 90.0, 0,0, 0,0 100.0 1.0 1.0 1.0 1.0 1.0	101 € 101 €

- Command dc rit
- Use of known format dectris. Header values are read.
 - Camera turned 270deg. Non-square detector is padded by zeros.
- The header scan values are wrong by 3% (Scan scale err 0.97)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.
- The several cycles to refine instrument model.



Dc rit: Diamond ID 19 Dectris turned II

at format				
Konun Cruskielan Imme	Песта	ers • and		
- North C Parts 10 Joints				
Generic uncompressed im	age			
Partierenter:	402	- (\$19.) (111)	Int JUNSIG SHORE CAN	INTES)
Frames info		5 12		
Run digits 🔄 0	Separator None	+ Frame 3	▼ name###.img	
C:\cryselepro_test\Exte	ernal_formats_Tacleusz\3004	diamond Wilatu	1_00001.dbf	
C:\crysalispro_test\Exta	enal_formats_Tadeusz13004	_diamond@ilatu\mp	1_00188.dbf Rrowne	3
		amport de	ta from headers	Run TC
eranto output				
mages base name:	mp1_00	Run #	1	
lotation [deg]: C o	C 90 C 180	· 270 C M	TOP	
hadandar tafa				
Posel size [mm]: 0.172	x0= 313.2 y	0= 323.6	> 000000.0 overfit	in l
and a second back				
Wavelength: USER		Ectif al1, nl2, h	Synchrotron	lambda
Monochromator:	MIRROR/SI	NORROTRON + H	Fact: 0.980 Edit	pollact
Alpha, Reta Ideol:	50.0.0.0	1	Edit	
Omena0 Theta0 Kann	0.0.0.0.0		Edit	
Onteger, means, rapp		Receiption of C		
Celector dec. fring:		Dearn Das Wis		51 H.L.
- Gom	and Michaeline		Pine det	
Scan Info	G Phi Omega- 0.0	Comerce	10.0	
and the	in the second second	- Concego	[main and a second sec	
Scarri start, step, expr	1.0, 1.0, 1.0	Theta	25.0 Kappa= 0.1	
Use tranes in inverse o	xder 1#86t, 2#86t-1	J Sca	n scale ent 0.970	Edit
Load Sav	-			
Load Sav				

Command dc rit

- Use of known format dectris. Header values are read.
- Camera turned 270deg. Non-square detector is padded by zeros.
- This data had NO scan scale error!
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.
- The several cycles to refine instrument model.



Dc rit: IPDS

Known Crysklafts format ● Generic uncompressed image Skip haader bytes: 1536 x=1200 y=1200 Post type STOE CHAR Frames into Run digts: III Separator Frame IIII namsFFF.ing D:\data\2014\3\Datan Mathias(\Virovetsi.jpdstast\\amov_010001.xi IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	pactorniat					
 Generic uncompressed image Skip haader bytes: 1536 x = 1200 y = 1200 Poet type STOE CHAR Frame's onto Run digits ■ Separator Runn ● Frame 3 ■ nameFFF.img D:\data\2014\3\Datan Nathias\\Virovets\ightatist\amax_010001.st D:\data\2014\3\Datan Nathias\\Virovets\ightatist\amax_010011.st D:\data\2014\3\Datan Nathias\\Virovets\ightatist\amax_010011.st D:\data\2014\3\Datan Nathias\\Virovets\ightatist\amax_010011.st D:\data\2014\3\Datan Nathias\\Virovets\ightatist\amax_010011.st D:\data\2014\3\Datan Nathias\\Virovets\ightatist\amax_010011.st D:\data\2014\3\Datan Nathias\\Virovets\ightatist\amax_010011.st Detector only.t Detector only Previous as (nm) 0.150. s0= 600.0 y0= 600.0 > 10000 > 100000 to 10000000000000000000000000000	C Known CrysAlisPro format					
Skip header bytes: 1536 x=1200 y=1200 Poel type STOE CHAR Prames info Run digits Separator Frame 3 nemeEFF;ing D'idata/2014/3/Daten Mathas//irovets/ipdsteet1/amox_010001.st Exercit did time tenter Exercit did time tenter D'idata/2014/3/Daten Mathas//irovets/ipdsteet1/amox_010156.st Exercit did time tenter Exercit did time tenter peranto output Exercit did time tenter Exercit did time tenter Exercit did time tenter peranto output Exercit did time tenter Exercit did time tenter Exercit did time tenter Paul acte (mm): 0.150 xb= 600.0 y0= 600.0 > 100000000000000000000000000000000000	Generic uncompressed im	oge				
Frames into Run digts Separator films Frame 3 maneffFring D:\data:\2014\3\Datan Mathias\\/inovets\ipdstect\\amov_010061.st D:\data:\2014\3\Datan Mathias\\/inovets\ipdstect\\amov_010156.st Event didt time tentor Peranto output peranto output peranto output Desctor infe Pixel size (mm): 0.150. xD = 600.0 yD = 600.0 > 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 > 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 > 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 > 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 > 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 > 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 S = 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 S = 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 S = 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 S = 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 S = 199958.2 Overflow Posel size (mm): 0.150. xD = 600.0 yD = 600.0 S = 199958.2 Overflow Posel size (mm): 0.0 682 Deam 0.000 688 Sam: 15.0 600 Sizen: 15.0 600 Sizen info@ Sizen info@ Sizen info@ Sizen isterf, step, esp: 0.0, 2.3, 100.0 Tuff Theta= 0.0 Kapper 0.0 @ Use frames in inverse order 1=last, 2=last-1 Sizen scale err 1.000 608 Sizen isterf, step, esp: 0.0, 2.3, 100.0 Tuff Theta= 0.0 Kapper 0.0 @ Use frames in inverse order 1=last, 2=last-1 Sizen scale err 1.000 608 Sizen Sizen isterf, step, esp: 0.0, 2.3, 100.0 Tuff Sizen isterf, step, esp: 0.0,	Skip header bytes: 1536	x	1200 y=	1200 Pixel	type STOE CHAR	11 - E
Run digits Iseparator Frame Image Prane Image Prane D:\data D:\data Image Prane Image Prane Image Prane D:\data D:\data Image Prane Image Prane Image Prane D:\data D:\data Image Prane Image Prane Image Prane Image Prane D:\data D:\data Image Prane Image Prane Image Prane Image Prane Prane Image Prane Image Prane Image Prane Image Prane Image Prane Prane Image Prane Image Prane Image Prane Image Prane Image Prane Prane Image Prane Image Prane Image Prane Image Prane Image Prane Prane Image Prane Image Prane Image Prane Image Prane Image Prane Detector info Image Prane Image Prane Image Prane Image Prane Image Prane Image Prane Where Image Prane Image Prane Image Prane Image Prane Image Prane Image Prane Monachromator: Image Prane Image Prane Image Prane Image Pr	Frames into					
D:\data\2014\3\Datan Mathias\\/irowts\ipdStestl\ama_010001.si Event D:\data\2014\3\Datan Mathias\\/irowts\ipdStestl\ama_010135.si Event peranto output mox Run # 1 Ratation (deg): 0 90 180 270 Merce Detector info mox Run # 1 Run # 1 Notation (deg): 0 90 180 270 Merce Detector info Morac 0.00 > 100000 > 1000000 00000 Pixel ease (mm): 0.120 x0= 600.0 y0= 000.0 > 1000000 00000 Vieweiength: MO 0.71, 0.71, 0.63 Control 10000 200000 Control 10000 Monachmeniatur: GRAPHOTE ELESPLANE divalue: 1.354 Edd divalue: 1.55 Scan: 15.0 Cont Edd Edd divalue: 1.56 Edd divalue: 1.56 Scan: 15.0 Cont Past Edd divalue: 0.00 Zat Edd divalue: Scan: 15.0 Cont Past 0.00 Zat Edd divalue:	Run digits 💌 🔋	Separator Incr	ні —	Frame 3	• namaH	∓.img
D:(data)2014/3/Daten Mathies(Virovet5/gddted11/amor_010156.x) Perento output perento output perento output Proges base name: amox Rus # Antation [deg]: 9 90 180 270 Merror Detector info Wavelength: MO 0.71, 0.71, 0.63 Circut1/citt Synchrotron Circut1/citt GRAPHITE ELESPLANE dvake: 1.354 Circut1 Comega0,Theta0, Kappa0 [deg]: 0.0, 0.0 Comega0,Theta0, Kappa0 [deg]: Comega Circut1	D:\data\2014\3\Daten N	athias/Wrowets	/.ijodstesti \amu	010001.M		TTAL B.
Periodic control Ban 1C periodic contput Brance Rule # 1 Rotation (deg): 0 90 180 270 Micror Detector info Phasi size (mm): 0.150 x0= 600.0 y0= 600.0 > 100000.0 100000.0 100000.0 100000.0 100000.0 1000000.0 1000000000000000000000000000000000000	D:\data\2014\3\Datan M	athias\Virovets	/ipdstest1\amo	C010156.M		units.
peranto output Droges base name: arrox Run # 1 Rotation (deg): 0 90 180 270 Microe Detector info Phuel ace (mm): 0.150 x0= 600.0 y0= 600.0 > 19998 0 overflow Deterument info Wowlength: M0 • 0.71, 0.63 CCCCCCC Synchrotron Fellowice Monochromator: GRAPHITE ELESPLANE • divake: 1.354 Edit divale Monochromator: GRAPHITE ELESPLANE • divake: 1.354 Edit divale Apho, Beta (deg): 50.0, 0.0 Cet Detector dist. (mm): 70.0 Cet Scan: 15.0 Cet Scan info Scan info Scan info * Use frames in inverse order 1=last, 2=last-1 Scan scale err 1.00 Edit Scan is in 1.00 Edit				The second	ala filoro finadora	Run TC
per on to output Dragges base name: amox Rut # Rotation [deg]: 0 90 180 270 Merger Detector info Pixel size [mm]: 0.150 x0= 660.0 y0= 600.0 > 1000000 > 1000000 1000000 Detector info Pixel size [mm]: 0.150 x0= 660.0 y0= 600.0 > 1000000 1000000 Volvelength: MO<	and the surface of					
Rotation [deg]: 0 90 180 270 Micror Detector info Pixel size [mm]: 0.150 x0= 600.0 y0= 600.0 > 1000000 Detector info Wowlength: MO 0.71, 0.71, 0.63 Cleatingth: Synchrotron Latingth: Wowlength: MO 0.71, 0.71, 0.63 Cleatingth: Synchrotron Latingth: Monachromator: (SRAPHITE ELESPLANE * drvake: 1.354 Edd drvake: Edd drvake: Apha, Beta [deg]: 50.0, 0.0 Coat Coat Detector dist. [mm]: 70.0 Cat Posal det. Lating Scan: 15.0 Coat Posal det. Lating Scan: Fhi Omegae 0.0 Coat Coat Scan: start, step, exp: 0.0, 2.3, 100.0 Tat Theta= 0.0 Kappa= 0.0 Edd V Use frames in inverse order 1=last, 2=last-1 Scan scale arr 1.00 Edd Edd	Images base name:	amox		Run #	1	
Norman (seg): s so 1 so 270 Marge Detector info Phasi size (mm): 0.150 x0= 600.0 y0= 600.0 > 1000000 > 10000000 Interpre Detector info Wowslength: MO • 0.71, 0.71, 0.63 CC2000000 > 1000000 Editional E	Ratative Televille	1 million	200 - C			
Detector info Pisal size (mm): 0.150 x0= 600.0 y0= 600.0 > 111111 overflow Inductioned info Wowlength: M0<	Rotation [deg]: 1• 0	90	0.180	270 M	mpr	
Pixel exe (mm): 0.150. x0= 600.0 y0= 00.0 > 19998.0 overflaw Intrument info Wowlength: M0 0.71, 0.71, 0.63 Executive: Synchrotron Executive: Manachromator: GRAPHUTE ELESPLANE divalue: 1.354 Edd divalue: Alpha, Beta [deg]: 50.0, 0.0 Edd Edd divalue: Omega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 Edd Edd Sam: 15.0 Edd Beam 0.00 Edd Scan: 15.0 Edd Pixel det. Edd Edd Scan: 15.0 Edd Demoga 0.0 Edd Scan: 15.0 Edd Comega 0.0 Edd Scan: 15.0 Edd Comega 0.0 Edd Scan: 15.0 Edd Comega 0.0 Edd Edd Scan: 15.0 Edd Comega 0.0 Edd	Detector info				and a present second in	
Detrument info Wowlength: M0 0.71, 0.63 Excellential Synchrotron Excellential Synchrotron Monochromistor: GRAPHUTE ELESPLANE divake: 1.354 Edd divake: Alpha, Beta [deg]: 50.0, 0.0 Edd Edd divake: Omega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 Edd Edd Detector dist. [mm]: 70.0 Ene Beam 0.00 Edd San: 15.0 Ene Beam 0.00 Edd Edd. Scan: 15.0 Ene Beam 0.00 Edd Edd. Edd. Scan: 15.0 Ene Beam 0.00 Edd Edd. Edd. Scan: 15.0 Ene Beam 0.00 Edd Edd. Edd. Scan: 15.0 Ene D.0 Gmega 0.0 Edd. Edd. Scan: 15.0 Ene 0.0 Gmega 0.0 Edd. Edd. Scan: Scan scale err 1.000 Edd. Edd. Edd. Edd. Scan: Scan scale	Pixel eze [mm]: 0.150.	×D=	600.0 y0=	600.0	> 99998.8	overflow
Mo 0.71, 0.63 COMMANDE Synchrotron Edit landet Manachromator: GRAPHITE ELESPLANE divalue: 3.354 68t divalue: Apha, Beta [deg]: 50.0, 0.0 64t 68t divalue: Omega0,Theta0, Kappa0 [deg]: 0.0, 0.0 64t 68t Detector dist. [mm]: 70.0 64t Beam 0.000 7dt Sam: 15.0 64t Pixel det. 67t Scan infor Scan infor Fhill Omegae: 0.0 68t Scan infor 0.0 10th Thetae 0.0 Scan istart, step, exp: 0.0, 2.3, 100.0 Tim Thetae 0.0 V Use frames in inverse order 1=last, 2=last-1 Scan scale arr 1.000 6dt	Instrument info					
Manachremator: GRAPHITE ELESPLANE d-value: 1.354 Edd d-value: Apha, Beta [deg]: 50.0, 0.0 Colt	Wavslength: MO	• 0.71, 0.7	1, 0.63	dit 415, 162, 10	Synchrotron	Edit lambde :
Apha, Beta [deg]: 50.0, 0.0 Celt Omega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 Celt Detector dist. [mm]: 70.0 Celt Sem: 15.0 Celt Scan infol Pixel det. Celtion Scan infol Scan start, step, exp: 0.0, 2.3, 100.0 Edt V Use frames in invorse order 1=last, 2=last-1 Scan scale err 1.00 cole	Monochromator:	- I	GRAPHITE ELE	PLANE · di	alue: 3.354	Edit divative
Omega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 Tdt Detector dist. [mm]: 70.0 Call Deam 0.000 Zdin Sean: 15.0 Call Posol det. Zdin Scan infg/ Scan infg 0.0 Gimega 0.0 Zdin Scan infg • Fhi Omegae 0.0 Scan infg 0.0 Scan infg 0.0 0.0 Scan: start, step, exp: 0.0, 2.3, 100.0 Title Theta= 0.0 Kappe= 0.0 V Use frames in inverse order 1=last, 2=last-1, Scan scale err 1.000 Ede Load Save Save Save Save Save	Alpha, Beta [deg]:		50.0, 0.0		Edit	
Detector dist. [mm]: 70.0 Enter Deam 0.000 Total Sam: 15.0 Enter Paul det. Enter Scan info; Scan info; Paul det. Enter Scan info; Fhi Omega 0.0 Scan; start, step, exp: 0.0, 2.3, 100.0 Titl Theta= 0.0 Kappie 0.0 If Use frames in inverse order 1+last, 2=last-1 Scan scale err 1.000 Edit	Omega0, Theta0, Kappi	0 [deg]:	2.0, 0.0, 0.0		Tdd	
Sem: 15.0 tott Phal det. Edition Scan http: Scan http: Scan; start, step, exp: 0.0, 2.3, 100.0 Tota Scan; start, step, exp: 0.0, 2.3, 100.0 Tota Voe frames in inverse order 1=last, 2=last-1 Scan scale err 1.000 tota Load	Detector dist. Immi:	20.0	-	Deam 0.0	00 1 75	
Scan infor Scan infor Scan: start, step, exp: 0.0, 2.3, 100.0 V Use frames in inverse order 1=last, 2=last-1 Load	Saint	15.0	-		Photi det.	T.ICO.
Scan type: • Fhi Omega 0.0 0	Scan min -	1999				
Scan: start, step, exp: 0.0, 2.3, 100.0 Tits Theta= 0.0 Kappa= 0.0	Scan type:	ie chi Omi	o.0	C Omega	0.0	
Scan, sent, s					0.0	100
Voe frames in myerse order 1=4ast, 2=4ast-1 Scan scale err 1.000	Scan; start, step, exp: 0	0, 2.3, 100.0		Theta=	0.0 Kappi	= 0.0
Load Contraction	IV Use traines in inverse of	rder 1=inst, 2=	-1868-1	Sca	n scale en: 1.	000 -666
	Load					

- Command dc rit/Import button on power toolbar
- Read detector information from the sum file of IPDS (0.15mm pix, cen x=600, y=600)
- Stoe char as pixel type; .xi files (this is OD compression...)
- Make sure to use resolution limit due to round IP image (Mo typical 0.809Ang)



Dc rit: IPDS 2

C Known CrysAlisPro format	¥
Generic uncompressed image	
Skip header bytes: 2560	x= 2267 y= 2267 Pixel type STOE CHAR V
Frames info	
Run digits 0 Separat	or None V Frame 4 V nameFFFF.img
Dildata)2014\12\inds_import[Ni	1984c 010001 vi
D:\data\2014\12\ipds_import\Ni	Le884C 010001.xi Browse
	Import data from headers Bun TC
neranto output	
Images base name: NLe8	84c_01 Run # 1
Rotation [deg]: (0 (90	0 C 180 C 270 T Mirror
Detector info, Auto-gap detection	
Pixel size [mm]: 0.1500	x0= 1133.0 y0= 1133.0
Use Auto-gap detection with vi	alue -1 Edu
Instrument info	
Wavelength: Mo 💌 0.	71, 0.71, 0.63 Edit al. al. b Synchrotron: 0.7107 Edit lambda
Monochromator:	GRAPHITE E1E3PLANE 💌 d-value: 3.354
Alpha, Beta [deg]:	50.0, 0.0 Edit
Omega0,Theta0, Kappa0 [deg]	: 0.0, 0.0, 0.0 Edit
Detector dist. [mm]: 60.0	Edit Beam 0,000 Edit
Gain: 15.0	Edit
Scan info	
Scan type: 🔿 Phi	Omega Phi= 0.0
Scan: start, step, exp: 0.0, 2.0,	10.0 Edit Theta= 0.0 Kappa= 0.0
Use frames in inverse order 1=	last, 2=last-1 Scan scale err 1.000 Edit
Load Save	

- Command dc rit/Import button on power toolbar
- Read detector information from the sum file of IPDS (0.15mm pix, cen x=1133, y=1133)
- Stoe char as pixel type; .xi files (this is OD compression...)
- Make sure to use resolution limit due to round IP image (Mo typical 0.809Ang)



Dc rit: dtrek frame from Japanese synchrotron

nout format		
 Xeron Continent Invest 	OTRES - music ced. elenus	
· · · · · · · · · · · · · · · · · · ·	forume Ti influences haven	
Generic incompressed image		
enter me	1024 ISBN 1024	7 KYTER;
Frames info		
Run digitz 💌 0 Separa	itor None 💌 Forme 3 💌 nameFFF.u	mg
Chevellowlate/2014/06/masks	Assemblighter and a STS Ma and SOIT me	
C:\acalitandata\2014\06\right	(serger/arean early SETS No. org 0007.ms	
		-
	and the second states and states	entities
Siperanto output		
Images bace name: K_B	ETS_Mo_org_0 Run # 1	
Rotation [deg]: (* p 👘 (*	40 (* 180 (* 270 (* Merer	
Detector info		
Posel stoe [mm]: 0.068	x0= 509.4 y0= 515.6	rfine
Distrument info		
Wavelangth:	🐨 Synchrotren	tot accute
Monactinametar:	MIRROR/SYNCHROTRON + Pollect: 0.500	Coll enther
Alsha Bata (deal):	90.8.0.0	
report onto [org]:		
Omegan, Frecan, Kappan (deg		
Detector dist. [rom]: 60.3	Besm 0.400 Besm	_
Gain: 15.0	C Poel det.	
Scan infu		
1967 C 1		
	10 10 10 10 10 10 10 10 10 10 10 10 10 1	8.81
Contract of the second se	Scan scale err 1,000	1000
		-
Last N Lost	8	

- Command dc rit/Import button on power toolbar
- The issue was here that the dtrek image was turn 90deg relative to the inhouse image. The dtrek createrunlist would not work on this.
- Thus the 'dc rit' command can be used to handly obstinate known images...



Dc rit: xpad detector

	Esperanto importer i	(1,0,3)
nput format		
Known CrysAlisPro forma	ESPERANTO -	
a anna linn anna an	11	
Generic Incumpressed in	unter processi processi	(1990-1) (2000-1000-100
Skip header bytes; 1290) <u>x=</u> 579 y= 562	Fixed type FLOAT (4 BYTES)
Trames info		
Ran digite 🛫 👘	Separator Pene	me - nameFFFF.dat
C:\xcel8urdata\2014\96	Flowenger/opted_img_02_0901.dnt	C. Contraction
C:/pcoliburdista/2014/de	Powengerlogad_ing_02_0001.me	Course
		Ans.
speranto output		
änages base name:	xped_img_	flun # 1
Rotation (deg): 🕫 D	C 90 C 180 C 270	E Mana
man and a start of the		2.0
Poul size Imml: 0.130	x0= 209.0 y0= 213.0	Co- more a overflow
Instrument info		Switchistran
westerigen. prov	Linconconcercitor	
Monochromator:	Manage Statements	Portice: 0.500
Alpho, Beta [deg]:	50.0, 0.0	
Omegab, Thetab, Kapp	s0 [deg]; 0.2, 0.7, 0.0	0.0
Detector dist. [mm]:	50.0 Bear	m 0.163
Gam:	1.0 0.0	🖓 Poel det. 👘 Let 14
Scan Infold		the second se
Scan Info	C Ma	Droege Phin 45.0
Scan info Scan type: Scan: start, step, cop: 2	C Me	Droege Phis 45.0 Theta= 32.0 Kappa= 10.0
Scan Info Scan type: Scan: start, step, exp: 2 Upe frames in inverse of	Ma	Drasge Phin 43.0 Thistoir 32.0 Kapper 10.0 Scan acale err 1.000
Scan infe(2 Scan type: Scan: start, stap, exp: -2 Use frames in inverse i	Pie 0.0 <td>Droege Phin 43.0 Thata= 32.0 Kappa= 10.0 Scan acale err 1.000</td>	Droege Phin 43.0 Thata= 32.0 Kappa= 10.0 Scan acale err 1.000
Scan Info Scan Info Scan: Idart, step, equ. 2 Upe frames in Inverse Scant	Pie 0.0 <td>Droege Phin 45.0 Theta+ 32.0 Kappa+ 10.0 Scan acale err 1.000</td>	Droege Phin 45.0 Theta+ 32.0 Kappa+ 10.0 Scan acale err 1.000
Scan Info Scan Info Scan: Idarf, step, expl. 2 Dise frames in inverse Scant Scan	Pie 0.0 0.0 00.0, 0.5, 10.0 2m 0.0 order 1 = back, 2=lask 1 0.0 0.0	Drosga Phis 45.0 Thata= 32.0 Kappa= 10.0 Scan acale en: 1.800

- Command dc rit/Import button on power toolbar
- The xpad detector is developed in France
- One of it's raw format can be channelled through the Esperanto importer
- As the header info is unknown, it has to be given in the scan info section.
- Provide the raw data file contains the -1 marker for pixel detectors the esperanto createrunlist command will automatically create a ccd file with dead zones.
- Such formats have to be transformed run by run as there is only one field for scan info.



Data finalization – optimal data

- Problems with...
- Experiment
- Unit cell
- Data reduction
- Finalization
- Pseudo symmetry, twinning, incommensurate



Experiment

- Problems with...
- Exposure time too low diffraction limit
- De-ice
- Movie missing
- Centering sample mount
- Choice of wavelength



Inspect executive tab

- Warning signs:
- Run list incomplete
- High mosaicity
- Scaling unusual
- I/sig low; low redundancy
- SG issues

Data Reduction

FRAMES/RUNS In run list: 402/7, used: 340/6

3D PROFILE ANALYSIS

Frames done: 340 Reflections tested: 2178, used: 1568 Avg mosaicity (in degrees) - 6 run(s) e1=1.10, e2=1.11, e3=1.31 Max incidence angle profile change(e3): 11% F)

3D INTEGRATION & FITTING

Frames done: 340 Fitted: 2231, overflow: 0, hidden: 15 Outliers rejected: 1

FINALIZATION INPUT FILE Filename: mm

FINALIZATION OUTPUT HKL FILE Filename: mm

SCALING / NUMERICAL ABSORPTION Empirical abs (e=2 o=0): min=0.99,max=1.01 Frame scales (1/scale): min=0.97,max=1.05 Friedel pairs treated as equivalent

RESULTS (340 frames) - SYM: Pmmm Resolution(A) Redundancy F2/sig(F2) Rint inf - 0.80 1.9 26.7 0.030 inf - 0.84 2.0 27.9 0.030 Completeness: 95.8% (0.84 ANG) Anom compl.: 83.6% (P222)

SPACE GROUP DESCRIPTOR P2(1)2(1)2(1) Group #: 19 (3 SG found) no data coverage: h00, 0k0,

DATA REDUCTION OPTIONS

Per-frame model refinement used 2-cycle 3D peak analysis used 3D profile fitting used



- Run 'Full auto analysis' on all data
- Concurrent may get stuck



Load new experiment Full auto analysis (cell, red) Automatic data reduction Data reduction with options

CrysAlisPro: Data reduction (1.13)

х



- Inspect frames
 - No diffraction at high angle \rightarrow cut the data to that resolution







- Inspect frames:
- Low/high background
- Diffuse scattering, split reflections, twin
- Empty frames, strange frames
- Inspect the sample movie (if you have it...):
- Sample mounting



Unit cell...

Ewald Explorer





Unit cell finding – Automatic unit cell finding







Unit cell finding – Influence of bad instrument model



Good instrument model



Bad instrument model:

Beam center deviation 40 pix





Unit cell finding – Influence of bad instrument model



Bad instrument model:

Beam center deviation 40 pix





Bad instrument model:

Delta-peak table



Unit cell finding – Influence of bad instrument model



Unit cell (twin vs. Jump)...









Unit cell (ice ring)...





Unit cell (filters)...





Unit cell (filters)...





Unit cell (filters)...



Ewald^{Pro} Collapse view

Collapse peak view – construction



- Lattice vectors are multiplied by lattice overlay size
- Subtract lattice vectors until given peak hits range



Ewald^{Pro} Collapse view



Ewald^{Pro} Collapse view

Collapse peak view – other examples



incommensurate



Data reduction

During experiment - concurrent data processing

 In most cases provides good, close to optimal results

- Features improving data quality:
 - Robust prediction model refinement
 - Selection of background evaluation mode





DATA REDUCTION OPTIONS Per-frame model refinement used 3D profile fitting used

no data coverage: 0k1, h01, h01, h00, 0k0,



Data reduction

Concurrent data processing - Robust cell / model refinement

- The key problem:
 - Inaccurate initial cell from pre-exp
 - Cell/Model can't predict well low/high theta
 - Misaligned/jumping sample
- Solution:

PROFFITPEAK module does standard peakhunting and cell/orientation refinement before profile learning / analysis phase




Data reduction

Concurrent processing - Automatic selection of background



Data reduction Use of lattice filters

Proffit: CrysAlisPro data reduction assistant (1.0.26)

CrysAlis

Profile fitting data reduction

Step 1: Orientation matrix for data reduction

UB - matrix:					
-0.016259	0.026962	0.037017 (0.000003	0.000004 0	.000006)
-0.018898	-0.024647	0.038739 (0.000003	0.000004 0	.000007)
0.027229	-0.000954	0.049096 (0.000003	0.000003 0.	.000006)
19.21287 (0.00171)	19.41060 (0.00194)	9.76017 (0.00089)
89.92280 (0.00771)	90.06198 (0.00728)	90.06002 (0.00764)
V = 3639.8	19				
elected cell (fr	com UM rr/UM	ttt/UM f):			
8 19.2129	19.4106	9.7602 89.9	228 90.062	90.0600	tI
Lattice extinctions	(filter Bravais la (P-lattice)	ttice extinctions)		nensurate structu ormal data reduct	res ion (HKL)
Use filter for:	He	uttice	- (S	ngle q-vector	Edit q m=0
				ther (reduction lief	Committee Land
			10	iner (reddcilon nsi	Generate Load
met a paras					
Lunning (Multion a	stal (activated b	y UM TWIN entri	es)		
i winning/mula crys	c twin/multi crvs	tal data reduction	n with the follow	ing components:	Multi crystei
Use automati					
Use automati	· · ·				
Use automati	nent1 🔲	Somponent 2	Compone	int 3 🛛 🦳 Comj	ponent 4
Use automati	nent1 🔲	Component 2	Compone	nt 3 🛛 🥅 Com	ponent 4
Use automati	nent1 🗖	Component 2	Compone	nt 3 🔲 Com	panent 4
Use automati	nent'i 🥅	Component 2	Compone	nt 3 🥅 Com	panent 4
Use automati	ment 1	Component 2	Compone	nt 3 🔲 Com	ponent 4



Data reduction Data reduction wizard

Settings worth attention:

- Model refinement options
- Special parameters:
 - Integration mask size
 - Bad profile filter
- Background options





Data reduction 3D profile fitting

- Distorted rotation method data is mapped to 'Kabsch-space'. Similar like XDS, but more complex
- Strong reflection data serve as reference profile. No shape assumption is made!
- All data is profile fitted to the 'nearby' reference profile. For strong data this means summation, for weak filtering
- You may choose to take less/more than 4sig of reference profile



Data reduction Special pars- outliers

- Filter intruders by correlation coefficient.
- All strong reflections are self similar.









Data reduction Special pars - incidence

 Profile fitting Override integration mask size (generally not recommended, but smaller mask can be useful for strongly overlapping reflections e.g. 1.00 of original size 	
Follow profile size changes with incidence angle	
Adjust masks according to prediction uncertainty (for high angle data)	
Print average profiles to history window	

Incide	nce	Т		Ave	rage	profile	size -	assumi	ng Gaussi	an shape	(in	degrees)		I
angle	(deg)	# of	peaks	Т	sig_e1	(stdde	v)	sig_e2	(stddev)	Т	sig_e3	(stddev)	I
		I			- -						I			- 1
0-1	2.6	I		769	I	1.639	(0.30	4)	1.430	(0.233)	I	1.757	(0.880)	I
12.7-1	8.1	Т		769	T	1.624	(0.35	4)	1.430	(0.242)	Т	1.649	(0.875)	I
18.1-2	2.5	I		769	Т	1.624	(0.35	7)	1.431	(0.258)	I	1.572	(0.828)	I
22.5-2	6.2	I		769	Т	1.594	(0.36	9)	1.414	(0.258)	I	1.542	(0.839)	I
26.2-2	9.9	I		769	Т	1.627	(0.37	2)	1.410	(0.282)	I	1.440	(0.736)	I
29.9-3	2.8	I		769	I	1.630	(0.36	4)	1.382	(0.255)	Ι	1.391	(0.719)	I
32.8-3	5.8	T		769	Т	1.594	(0.34	1)	1.341	(0.267)	I	1.392	(0.708)	I
35.8-3	8.9	T		769	Т	1.632	(0.34	9)	1.337	(0.266)	I	1.315	(0.594)	I
38.9-4	1.9	T		769	Т	1.638	(0.33	0) I	1.294	(0.269)	I	1.303	(0.659)	I
41.9-5	1.6	T		769	Т	1.618	(0.32	3)	1.221	(0.270)	I	1.188	(0.610)	I
		T			- 1 -			1			1			- 1
0-5	1.6	Т		7690	1	1.622	(0.34	7)	1.369	(0.269)	I	1.455	(0.769)	I

Profile size analysis (per incidence angle)

Fitted profile normalization line parameters

e1 dimension: a=0.0022 b=0.99

e2 dimension: a=-0.0019 b=1.08

e3 dimension: a=-0.0136 b=1.46



Data reduction Prediction uncertainty – problem

- Problem lies in spot prediction uncertainty
- Higher inaccuracy at high theta



For profile size of 0.8 deg integration mask size is 8 pixels at incidence angle 0 deg (Atlas detector, 2x2 binning, at 55 mm)

Detector theta (deg)	Std dev of misprediction (deg)	Std dev of misprediction (pix)	Max misprediction (pix)
11	0.014	0.13	0.78
24	0.02	0.2	1.2
40	0.025	0.25	1.5
111	0.04 - 0.08	0.4 – 0.8	2.4 – 4.8



Data reduction Prediction uncertainty – solution

• Estimate prediction uncertainty at given theta

Prediction ac	curacy statist	ic	s (in degrees)					
1			Average predic	tio	on error (in degrees))		
Resolution	# of peaks	L	delta_e1 (stddev)	Τ	delta_e2 (stddev)	Т	delta_e3 (stddev)	
		L		1		I.		- I -
1.35-1.22	82	L	0.002 (0.020)	1	0.001 (0.013)	Т	0.003 (0.170)	1
1.22-1.14	82	L	-0.002 (0.025)	1	0.009 (0.016)	Ι	0.020 (0.165)	
1.14-1.08	82	L	0.003 (0.024)	1	0.004 (0.020)	Т	0.020 (0.175)	
1.08-1.04	82	L	-0.012 (0.034)	1	-0.002 (0.021)	Т	-0.026 (0.153)	
1.04-0.99	82	Ι	0.001 (0.026)	T	-0.003 (0.021)	Ι	-0.018 (0.153)	
0.99-0.95	82	L	-0.007 (0.033)	1	-0.005 (0.030)	Т	-0.004 (0.147)	
0.95-0.91	82	L	-0.005 (0.038)	1	-0.009 (0.029)	Τ	-0.001 (0.132)	
0.91-0.87	82	L	-0.008 (0.038)	T	-0.015 (0.041)	Ι	-0.002 (0.127)	
0.87-0.84	82	I	0.006 (0.038)	T	-0.012 (0.041)	Τ	-0.016 (0.106)	
0.84-0.80	73	L	0.005 (0.051)	1	0.017 (0.087)	Τ	0.002 (0.103)	
		L		Ι		Τ		1
1.35-0.80	811	L	-0.002 (0.034)	- i	-0.002 (0.038)	Ĩ.	-0.002 (0.146)	Ì.

• Enlarge integration mask according to prediction uncertainty



Data reduction Model refinement options



Data reduction Model refinement options







Data reduction Model refinement options





• For discontinous sample jumps (LT, flexible holder, not fixed properly, etc.)









Sample slippage example

- Superficially gives impression of twin
 - Twin indexing matches 96.8% of reflections

TWIN ANALYSIS Ratio Isolated Overlapped Component 0.37 1676 24 0.63 1690 2 24 DECOMPOSED TWIN DATA STATISTICS (<0.80 overlap) Component Redundancy F2/sig(F2) Rint 1.5 9.7 0.245 1.5 7.0 0.658 Overlap limit for HKLF4 export: 0.80 TWIN HKLF5 STATISTICS FOR OVERLAPPED OBS Components Redundancy F2/sig(F2) Rint 1.2 24.8 0.223 1.3



... but twin integration doesn't help



Sample slippage example





Sample slippage example







Sample slippage example



	No slip	Intentional sample slip				
	Reference data	Slip Data (Pre- Treatment)	Slip Data (Post- Treatment)			
R _{int} (%)	1.6	14.7	1.6			
/σ	22.0	5.0	22.9			
R ₁ (%)	3.32	43.88	3.46			
Comp (%)	98.5	95.2%	98.4%			



Background correction

				CrysAli
p 4: Background	evaluation			
Background for 3	D centroids			
For an acurate ev parameters contr	valuation of integrated ol this evaluation: The	intensities a good backgroun evaluation range Re and the	id determination is es repeat frequency Fr.	sential. Two
Re = 25	Edit Re	Fr = 25 Edit Fr		
Binning may redu or 4 in case of lac	ce the memory requir k of physical memory C 4 I R nemory space for bac	ements for the background ev on your machine (risk of swap educe background accumula kground evaluation: 189.8/50.	valuation, Default is 1. pping)! ttion to SHORT type (0 Mb	You may use 2 saves memory)
Background for 3	D integration	troid evalutation (good for sta	ble & low background	d, fast)
Background for 3 C Average ba C Smart backg with high back	D integration ckground from 3D cen ground (combination o skground and locally v	troid evalutation (good for sta f local and average backgrou arying features, e.g. protein d	ble & low backgroun und computation, goo lata, slower)	d, fast) d for weaker data

Choice of background correction:

- Average background
 - Define range and frequency
- Smart background
 - Combination of local and average background
 - Improves statistics (I/σ) for samples with varying background features



Background correction



Well-mounted sample

Standard peak-hunting produces many non-lattice peaks.







Intentionally badly-mounted sample

Background correction



	Well- mounted	Badly-	mounted		
	Reference Data	Auto analysis	Smart Background		
Time	3h 8m	16h 18m	16h 18m		
Diff. Limit	0.92	1.41	0.97		
R _{int} (%)	3.1	14.4	5.8		
l/σ	13.5	3.0	7.8		
R ₁ (%)	5.28	-	6.22		
Comp (%)	99.5	99.5	99.5		



Manual Data Reduction Bad profile rejection



Simulation of cryo-failure (shield flow turned off)





Bad profile rejection



No ice		arge ice build	-up
Reference Data	Auto analysi s	d range and run Filtering	Bad profile filtering
2.6	10.5	3.2	4.0
17.7	8.4	14.0	12.7
3.83	6.11	4.11	4.50
99.9	99.9	92.6	98.6
	No ice Reference 2.6 17.7 3.83 99.9	No iceAuto analysi analysi sReference DataAuto analysi analysi s2.610.517.78.43.836.1199.999.9	No iceAuto analysi sd range and run FilteringReference DataAuto analysi sd range and run Filtering2.610.53.217.78.414.03.836.114.1199.999.992.6



Manual Data Reduction XX PROFFITLOOP - ultimate tool

 Not satisfied with the results, consider trying different option combinations using PROFFITLOOP tool

	Proffit loop dialog
Proffic CrysAlsPro data reduction assistant (10.26)	General options
	Follow sudden (discontinuous) changes of sample orientation
Profile fitting data reduction CrysAlis	Follow profile size changes O Yes O No Doth
Step 1: Drientation matrix for data reduction	Adjust masks according to prediction uncertainty • Yes No Both mask
78 - 4465184 -0.001365 0.189652 -0.00813 (0.000000 0.000000 0.000000) 0.001365 0.1896555 0.10196 (0.000000 0.000000 0.000000)	Override mask size O Yes No Both 1.00
5.054479 5.00122 -8.582541 (0.00000 6.50000 6.50000 6.50000 7 8.5642 (0.0000 9.57005 1 0.0000 0 13.45858 1 0.0000 7 85.95511 8.5000 9 68.38422 (0.0000 7 85.54212 (0.0000 7	Smart background C Yes No Both 1
Neinensed voll. (drawn Thir ray/Thir con/Thir (d)) 102 6. Seret 6. 2000 1.0. 1040 100.0000 10.0000 10.0001 10.0001 10.0001	Use short r
Note analyse found P-Lettion in peak humbing data!	Additional info
Latice solucions (Mer Bravas Mice editcions) Incommensurate douctures	Addition file info
C Use (Restor	Summary
C OPer (reduction list)	Number of loops to complete calculations: = 1
Twinning/Multi crystal (activated by UM TWIN entires)	Sample file name:
[10] Construction of the state of the sta	pre_exp_2315_pl_mask
Eest Bext - Finan Cancel Heip	Note: the following dialog generates only the script with all selected options. In order to start computations type SCRIPT in command line and select PROFFITLOOP.MAC file.



Caution! This tool may run for a long time and generate a lot of output files with gibberish names





Manual Data Reduction XX PROFFITLOOP - ultimate tool

• Afterwards browse the results in the finalizer window

Data reduction 1	file contents	Data re	duction output	1	Red grap	dis	Data collection	output	Device	es log
105-2 04	20	40	26			2702146 02	00.20	0.007	0.010	
1HI-2.04	29	40	26	65 0	1.4	1647384 02	60.85	0.007	0.010	
2.32-1.99	27	50	26	52.0	1.0	1143713.65	37.95	0.041	0.015	
1.98-1.82	35	37	26	70.3	1.3	693092.30	32.82	0.013	0.026	
1.82-1.69	30	51	26	51.0	1.2	680136.67	24.54	0.016	0.023	
1.68-1.56	2.6	51	26	51.0	1.0	663546.27	22.14	0.000	0.000	
1.56-1.47	28	52	26	50.0	1.1	597198.54	20.00	0.029	0.040	
1.47-1.41	27	57	26	45.6	1.0	391726.23	15.04	0.048	0.053	
1.40-1.34	27	59	27	45.8	1.0	305305.47	13.30	0.000	0.000	
1.33-1.26	26	89	26	29.2	1.0	386551.82	14.75	0.000	0.000	
inf-1,26	291	537	261	48.6	1.1	948740,98	34.27	0.010	0,014	
inf-2.84	30	42	25	40.5	1.2	2779347 65	94 61	0.004	0,009	
2.83-2.17	46	38	25	65.0	1.8	1451383.82	68,79	0.011	0,011	
2.15-1.90	39	36	25	69.4	1.6	963106.64	44.19	0.014	0.016	
1.89-1.73	36	35	25	71.4	1.4	542996.56	25.45	0.040	0.031	
1.72-1.56	35	41	25	61.0	1.4	701577.69	29.48	0.030	0.028	
1.55-1.46	32	41	25	61.0	1.3	539831.23	21.38	0.028	0.032	
1.45-1.36	35	45	25	55.6	1.4	402046.47	17.89	0.018	0.036	
1,35-1.26	38	68	32	47.1	1.2	340238.39	15.65	0.027	0.041	
inf-1.26 Data reduct	291 tion ende	351 d at Wed	207 Mar 18 12:	59.0 21:33 2	1.4	948740.98	39.79	0.015	0.017	
Refinalize	Crystal mo	vie			aca 211	5 cl. mask		7		
Contraction of the local division of the loc	-	Marie Contraction			120,21	o primask	(CALLS)	1		



Post-integration empirical corrections

- Scaling
- Empirical absorption based on spherical harmonics
- Decay
- Detector sensitivity

alization dialog: SM exp	hkl-file:C:\XcaliburData\exp_2315\exp_2315.hkl	
	Output dir C:\CaliburData\exp_2315	
🚌 🚽 🖌 Finali:	Symmetry settings	rvsAl
Sample	✓ Use Friedel mates as equivalent even for noncentrosymmetric SG	
Experiment: exp_2315	LS refinement control	
Set formula:	SigCut: 7.00	
Corrections Empirical correction	Exclude 15 strongest unique reflections (along with all symmetric equivalents)	
Frane scaing:	Frame scaling B-factor/A-factor refinement	-115
 Sample decay 	Automatic frame scale assignment V Apply frame scaling Refine B-factors	Rector and a
Numerical absorption	How many frames have 4 frames = 1 scale	
Space group and AutoChe Search for space group	Variation restraint (ESD): 0.20000	oup options
AutoChem	✓ Reject frame scales 0.20 & > 5.00 Westraint 0.20000	m options
Filters and limits	- Empirical shearstion correction	
Automesea	Automatic parameter selection for absorption correction	
Output	Have such as the second of the address of the second of th	
Standard set of		Change
Oreate/overwrite exp_3	Absorption correction before frame scaling (recommended for strong absorbers)	
Lipott aptions	Detector area scaling	
	How many detector area regions? 4x4 Apply detector correction	3
	Variation restraint (ESD): 0.20000	Cance

Try manual settings!





Remark on scaling of non-centro data

- Organic samples Friedel pairs equivalent
- Samples with heavier atoms

 scaling with Friedel pairs
 merged may destroy
 anomalous signal info
- Version 38 makes automatic decision based on provided formula ("heavy" means Si for Cu, Sc for Mo)

Output dir C:WcaliburData\exp_2315 ry settings re Friedel mates as equivalent even for noncentrosymme	etric SG
SigCut: 7.00 Exclude 15 strongest unique reflections (along with	h all symmetric equivalents)
Frame scaling Image: Automatic frame scale assignment Image: Apply frame scaling How many frames have a common scale? 4 frames = 1 scale Variation restraint (ESD): 0.20000 Image: Reject frame scales 0.20 & > 5.00	B-factor/A-factor refinement Refine B-factors Refine A-factors 10 frames = 1 factor Restraint
Empirical absorption correction Automatic parameter selection for absorption correction Max even order: 8 Max odd order: 0 Absorption correction before frame scaling (recommended for se	 44 parameters trong absorbers)
Detector area scaling How many detector area regions? 4x4 v A Variation restraint (ESD): 0.20000	pply detector correction



Optimal data – hints at experiment time

- Centering/Sample choice/holder/amount of oil
- Low T: de-ice runs
- Absorption: make movie 1-6 deg
- Concurrent data red re-start
- Cu Mo choice
- Collect redundant data
- Rather reduce scan width than increase dd
- Check your diffraction limit



Optimal data – hints at unit cell finding time

- Check for non-indexing reflections
- Garbage (ice rings, powder), twin, sample jump
- Re-run refine model
- Ewald
- Use filters (intensity, lattice type) and groups
- Use intensity view
- Check chemical formula unit cell consistency



Optimal data – hints at data reduction time

- Check for experiment artifacts (empty frames, trips)
- Apply Bravais lattice where obvious
- Special pars
- Use bad reflection filter
- Use reduced profile size if overlapping
- Incidence correction, prediction accuracy
- Smart background on high background data
- xx proffitloop



Optimal data – hints at data finalization time

- Hand set empirical parameters
- Use shape based absorption correction
- Apply filters carefully (e.g. Rint)
- Interactively decide space group
- Remove unnecessary data via d-value filter



Software Updates

- CrysAlis^{Pro} is frequently updated with fixes for known problems
- New features are introduced in annual major updates
- All updates are *Free* and available from our user forum, http://www.rigakuxrayforum.com
- Free multi-user, multi-site license

Rigaku						
			& Portal	P Search	🗂 Calendar	E 164
elcome back, mathias meyer. You last sisted: 05-06-2015, 02:	12 PH Log Out 🗝					Search
k meer car	Open Buddy List	Vev New Fasts	View Today's Post	te: Private M	eseper (Drews)	II, THEFT
igalui Oxford Diffraction forum						
Announcements:						
inun .		Three	és Posts		Last Part	
General Updates Other inve		36	38		Support relate 16-06-301	C Desgenet S, NG-07 W
Suffware Develop, get help with, and stocers activers Such forces to parage cognitistive Download						•
nege en la contra de la contra de Ferenaria		These	a. Pests		Last Part	
CrystAlisPro a Sab totam for the CrysVePra software totaling develoads, menual tech Prevent: * Deveload CrysVePra, * Decase Crystalistic, and	, grides and deconsises around 2 maris	378	L365		operation control sector 19-cm control by perat	to noce. 5, 68:13 M
CrystalDyrs The next version of CrystalDyre for the VX Science Sele Provide:	3 mire.	1	1		Demonstra 20-es-con ky	tions wideo 5, ozulta et Transr tittet
Other third party software A place to denote and pet hile with non-Ripile orthogen.		0	. 0		Never	
lieneral Crystalligraphy A ne peded wedfe term for cyclolography disarraw of pace groups, o		erer yna hany				4
1414 1		three	ds Posts		Last Past	
Applications A farm for Annatory applications and factoriages Selt Provide: # Small Melecule, # Printer		129	eis		19-96-201	5, 12:13 Ph By Astronomy
Conferences, Exhibitions, and Pressentations West conferences will be attending, and growintations will great.						
Course -		Three	ds Posta		Last Past	
Uterwaters, Posters and Presentations Links & Developh to application miss, anders and presentations from Sale foreases: A Uterwise Users, A Presentations	s varlaus conferences	8	24	8	tanapeon X cay ((B+0+0)0 by)	rystallog. 5, nexts Ar
Conferences and Exhibitions Internet points		1	1		0pt	1 ILD A



Thank you for listening!

Find out more at

www.rigaku.com

