https://bl831.als.lbl.gov/~jamesh/powerpoint/RapiDataXDStutorial_2025.pptx

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Useful links

← → C (the https://bl831.als.lbl.gov/~jamesh/powerpoint/?C=M;O=D

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Index of /~jamesh/powerpoint

	Name	Last modified	Size Description
J	Parent Directory		-
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?	<u>RapiData_XDStutorial></u>	2024-04-30 09:21	1.5M
B	fear_no_Spacegroups.mp4	2024-03-13 13:47	326M
Ē	fear_no_Spacegroups.pdf	2024-03-13 09:38	6.9M
?	fear_no_Spacegroups>	2024-03-12 20:27	106M
?	<u>Ringberg_tangle_2024></u>	2024-02-15 05:54	7.0M
?	SIBYLS_tangle_2024.pptx	2024-01-08 11:38	6.0M
?	MX_at_ALS_JMH.pptx	2023-12-04 21:18	10M
_	-		

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Chapter 7: Tips and Tricks

Neat-o unix commands

: is the little sentence you type to run unix programs. The text that appears on each line to the left of e command prompt. This is a very old convention, but it is incredibly powerful. No graphical close to providing the detailed control that a command line gives you. The only problem with hey almost always have obtuse syntax, and novice users have a really hard time figuring out what to ended as a quick guide for crystallographers who want to optimize their unix environment without all the unix manuals that I have. :)

he unix "shell"

Your "shell" program is probaly tesh (Turbo-C-shell). All a shell program does is accept your typed commands, find and run the unix program you have invoked, and then prompt you for another command. That's about it. However, the shell is



Main page Recent changes Random page Help about MediaWiki

Page Discussion Read View

Difficult datasets

The following suggestions apply not only to or low-resolution, or otherwise difficult macromolecular gatasets

These datasets have few (or few strong, or few well-defined) reflections per frame. Therefore, the multitude of parameters describing the diffraction experiment needs to be reduced (in refinement one would say: to avoid overfitting). This means that some

Fear no Space Groups





James Holton's Benchmarks...

Comparison of x-ray programs on different machin

The following tables are a comparison of standard x-ray data-processing access to. The machine names have been omitted to protect the innocent. "major" process on the machine, and always from a local disk. The exact moved from machine to mahcine.

Speed of DIALS



Log in

XDS

X-ray diffraction data reduction engine

Diffraction image data

Adxv - trp_ag_0001.cbf _ 🗆 🛪													
and the second for the second													



List of spot intensities (text)

	Open 🔻	Æ			(/de	(DS_ASCII ev/shm/james	.HKL h/bench	
ľ	!DIRECTION	0F_[DETEC	TOR_Y-AXIS=	0.00000	1.0000	0 0.00	000
	!VARIANCE	MODEL	_= 9	0.618E-01 2	.594E-04			
	!NUMBER_0	F_ITEM	4S_IN	LEACH_DATA	RECORD=12			
	!ITEM_H=1							
	!ITEM_K=2							
	!ITEM L=3							
	!ITEM IOBS	5=4						
	!ITEM SIG	MA(IOE	BS)=5	5				
	!ITEM XD=0	5						
	!ITEM YD=7	7						
	!ITEM ZD=8	В						
	!ITEM RLP=	=9						
	!ITEM PEAK	<=10						
	!ITEM COR	R=11						
	!ITEM PSI=	=12						
	!END OF HE	EADER						
	-0	0	1	-4.155E-01	4.271E-01	1323.0	1256.5	24
	Θ	0	1	2.890E-01	4.948E-01	1323.0	1208.6	26
	Θ	0	1	2.898E-01	4.947E-01	1323.0	1208.6	22
	Θ	0	1	2.899E-01	4.941E-01	1323.0	1208.6	18
	Θ	0	1	-4.165E-01	4.266E-01	1323.0	1256.5	20
	Θ	0	1	2.897E-01	4.947E-01	1323.0	1208.6	33
	Θ	0	1	-4.155E-01	4.264E-01	1323.0	1256.5	35
	Θ	0	1	-4.162E-01	4.269E-01	1323.0	1256.5	31
	Θ	0	1	-4.157E-01	4.273E-01	1323.0	1256.5	27
	Θ	0	1	2.919E-01	4.946E-01	1323.0	1208.6	29
	Θ	0	1	-4.188E-01	4.267E-01	1323.0	1256.5	6
	Θ	0	1	2.896E-01	4.942E-01	1323.0	1208.6	8
	Δ		1 -			1000 A	-1-70.0 6-	/
						Plain lext	 lab Wi 	atn:

XDS

native user interface: a text file!

Open 🔻	XDS.INP ~/xds_tutorial	Save = -		×							
! written by generate_XDS.INP version 0.82 (0 JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGP ORGX= 1231.50 ORGY= 1263.50 ! values from fr	1-Mar-2018) ATE CORRECT Tame header; only read by X	CORR, IDXREF									
DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to crystal. OSCILLATION_RANGE= 0.2000 STARTING_ANGLE= 270.0000 X-RAY_WAVELENGTH= 0.97946 NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_????.cbf ! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing DATA_RANGE=1 1800 SPOT_RANGE=1 1800 ! BACKGROUND_RANGE=1 10 ! rather use defaults (first 5 degree of rotation) SPACE_GROUP_NUMBER=0 ! 0 if unknown											
SPACE_GROUP_NUMBER=0 ! 0 if unknown UNIT_CELL_CONSTANTS= 70 80 90 90 90 90 90 ! put correct values if known INCLUDE_RESOLUTION_RANGE=50 0 ! after CORRECT, insert high resol limit; re-run CORRECT ! IDXREF now obeys INCLUDE_RESOLUTION_RANGE and EXCLUDE_RESOLUTION_RANGE to exclude ice-rings											
FRIEDEL'S_LAW=FALSE ! This acts only on t ! If the anom signal turns out to be, or is k ! use FRIEDEL'S_LAW=TRUE instead (or comment	he CORRECT step nown to be, very low or ab out the line); re-run CORRI	sent, ECT									
<pre>! remove the "!" in the following line: ! STRICT_ABSORPTION_CORRECTION=TRUE ! if the anomalous signal is strong: in that ! "CHI^2-VALUE OF FIT OF CORRECTION FACTORS"</pre>	case, in CORRECT.LP the the values are significantly> :	ree l, e.g. 1.5									
<pre> ! exclude (mask) untrusted areas of detector, ! UNTRUSTED_RECTANGLE= 1800 1950 2100 2150 ! ! UNTRUSTED_ELLIPSE= 2034 2070 1850 2240 ! x- ! UNTRUSTED_QUADRILATERAL= x1 y1 x2 y2 x3 y3 !</pre>	e.g. beamstop shadow : x-min x-max y-min y-max ! min x-max y-min y-max ! if x4 y4 ! see documentation	repeat needed									
! parameters with changes wrt default values: TRUSTED_REGION=0.0 1.2 ! partially use corner	s of detector (0 1.4143: us	se all pixels) An is ok									



avigation

- Main page
- Recent changes
- Random page
- Help about MediaWiki

earch

Search XDSwiki										
Go Search										
ols										
What links here										

- Related changes
- Special pages
- Printable version
- Permanent link
- Page information

page discussion

view source

e history

Generate XDS.INP

This script generates XDS.INP based on a list of frame names supplied on the commandline. It currently works for MarCCD, ADSC, Pilatus, Eiger, some Rigaku and one Bruker detector(s); since this is just a bash script, extension to other detectors should be very easy.

log in request account

	Contents [hide]
1	Usage
2	The script
3	System-wide or personal installation
4	Copying generate_XDS.INP from XDSwiki webserver
5	Obtaining generate_XDS.INP from this webpage
6	Calling generate_XDS.INP from a Python script
7	Dependencies
8	Limitations

Usage

9 See also

Usage is just (don't forget the quotation marks!):

generate_XDS.INP "/home/myname/frms/mydata_1_???.img"

XDS supports d bzip2-ed frames. Thus, when specifying the frame name parameter of the script, you should leave out any .bz2 extension.

A better image viewer

🗙 Adxv	× +				\sim	—	×
← → C	https://www.scripps.edu/tainer/arvai/adxv.html	Ŕ	☆	<mark>الم</mark>	4	*	:

Adxv - A program to display X-Ray diffraction images

Adxv can be used to display and analyze 2-D area detector data. It is optimized to display X-Ray crystallography diffraction images. The data may be displayed as a 1-D cross section, 2-D image or 3-D surface. Sequential images may be displayed as an animation. The magnification, contrast and color mapping are adjustable. Displayed data may be saved in a variety of formats including ASCII, SMV/IMG, TIFF, JPEG and Postscript. Adxv will run on most versions of Linux and OSX. It is based on X11/Motif so an X-server is required. It will run on Windows if the Cygwin libraries and X-server have been installed.

Many common detector and data formats are recognized, including:

- ADSC
- Mar ccd
- Mar image plate (old and new format)
- Raxis II & IV
- Crystallographic Binary Format (CBF)
- XDS .pck files
- European Data Format (EDF)
- Numerical Python (NUMPY)
- Hierarchical Data Format (HDF5)
- Tagged Image File Format (TIFF)
- Raw binary integer and floating point data



XDS native user interface

	📃 🚳 📃 🖳		
	Terminal -	↑ _ □ ×	
File Edit View T smbnxs3:~> pxp	erminal Tabs Help roc dialog.sh	1	
	Open new shell on	↑ □ ×	
	Terminal -		↑ _ □ ×
File Edit View Terminal	Tabs Help		
<pre>pxprocl2:~> cd xds_t pxprocl2:~/xds_tutor '.cbf generate_XDS.INP ver http://strucbio.biol DATA_RANGE=1 1800 Data from a Pilatus STARTING_ANGLE= 270. ORGX= 1231.50 ORGY= DETECTOR_DISTANCE= 1 OSCILLATION_RANGE= 0 X-RAY_WAVELENGTH= 0. XDS.INP is ready for Full documentation, http://www.mpimf-hei After running xds, i BKGPIX.cbf, and the pxprocl2:~/xds_tutor [1] 72219 pxprocl2:~/xds_tutor</pre>	<pre>utorial ial> generate_XDS.INP /data sion 0.82 (01-Mar-2018) . 0 ogie.uni-konstanz.de/xdswik detector 0000 1263.50 - check these value 89.16000 ! only read by XYC .2000 ! only read by IDXREF 97946 ! only read by IDXREF use. The file has only the including complete detector delberg.mpg.de/~kabsch/xds nspect, using XDS-Viewer, a agreement of predicted and ial> gedit XDS.INP & ial> xds_par</pre>	/holton/demo/lyso1_18 btain the latest vers i/index.php/generate_ s with adxv ! ORR, IDXREF most important keywo templates, is at . More documentation t least the beamstop observed spots in FRA	39mm_1_'????? sion from _XDS.INP ords. in XDSwiki mask in AME.cbf!



Mouse

can be used To select and paste But all pasted text Goes to the cursor



- 1) Make sure X11 is running
- 2) Select some text with mouse
- 3) Move mouse over to your terminal
- 4) Hit middle mouse button
- 5) No keyboard required!

How to start XDS



xdsgui – a graphical interface for XDS

9					0	T5 XDSGUI	2020-12-0	2 running in /mr	nt/home1/rapio	data3/xds	_tutorial		
<u>/</u> enu He <u>l</u>	С												
Projects	Frame	XDS.INP	XYCORR	INIT	COLSPOT	IDXREF	DEFPIX	INTEGRATE	CORRECT	tools	statistics	XDSCONV	XSCALE
Folder v	vith XDS o	configur	ation and	loutpu	ut files								
Default is	the current	directory.	The title ba	ar of the	e XDSGUI wir	ndow show	s the curre	ntly used folde	r.				
			Load rece	ent proje	ect								
Choose	or create ne	ew folder											

xdsgui – load an image



xdsgui – a GUI for text!

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds tutorial Menu Help XDS.INP Projects Frame XDSCONV tools statistics XSCALE Save Run XDS ! written by generate XDS.INP version 0.82 (01-Mar-2018) JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT ORGX= 1231.50 ORGY= 1263.50 ! values from frame header; only read by XYCORR, IDXREF DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to crystal. OSCILLATION RANGE= 0.2000 STARTING_ANGLE= 270.0000 X-RAY_WAVELENGTH= 0.97946 NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/1rb5_1_????.cbf ! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing DATA RANGE=1 1800 SPOT_RANGE=1 900 ! BACKGROUND_RANGE=1 10 ! rather use defaults (first 5 degree of rotation) SPACE GROUP NUMBER=0 ! 0 if unknown UNIT_CELL_CONSTANTS= 70 80 90 90 90 90 90 ! put correct values if known **INCLUDE RESOLUTION RANGE=50 0** ! after CORRECT, insert high resol limit; re-run CORRECT ! IDXREF now obeys INCLUDE RESOLUTION RANGE and EXCLUDE RESOLUTION RANGE to exclude ice-rings FRIEDEL'S_LAW=FALSE ! This acts only on the CORRECT step ! If the anom signal turns out to be, or is known to be, very low or absent, ! use FRIEDEL'S LAW=TRUE instead (or comment out the line); re-run CORRECT ! remove the "!" in the following line: ! STRICT_ABSORPTION_CORRECTION=TRUE ! if the anomalous signal is strong: in that case, in CORRECT.LP the three "CHI^2-VALUE OF FIT OF CORRECTION FACTORS" values are significantly> 1, e.g. 1.5

XYCORR- setting things up

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial													
M	enu He <u>l</u> p												
F	Projects Frame	XDS.INP	XYCORR	INIT	COLSPOT	IDXREF	DEFPIX	INTEGRATE	CORRECT	tools	statistics	XDSCONV	XSCALE
						S	ave				Run XDS		
	JOB= XYCORR ORGX= 1231.50 ORGY= 1263.50 ! values from frame header; only read by XYCORR, IDXREF												
	DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to crystal.												
	DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359 !PILATUS												
	SENSOR_THICK	NESS= 0.3	32 97946										
	NX= 2463 NY-	2527 Q	(= 0.172	QY=	0.172 ! t	to make (CORRECT	happy if fr	rames are	unava	ilable		
	NX= 2463 NT= 2527 QX= 0.172 QY= 0.172 ! to make CORRECT happy if Trames are unaVailable OSCILLATION_RANGE= 0.2000 !STARTING_ANGLE= 270.0000 DIRECTION_OF_DETECTOR_X-AXIS=1 0 0 DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0												

INIT – look at the background

		C	QT5 XDSGU	1 2020-12-02	2 running in /mn	t/home1/rapid	data3/xds	_tutorial					
Menu Help													
Projects Frame XDS.INP	XYCORR INIT	COLSPOT	IDXREF	DEFPIX	INTEGRATE	CORRECT	tools	statistics	XDSCONV	XSCALE			
	Save Run XDS												
JOB= INIT													
DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to crystal.													
NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_????.cbf													
DATA_RANGE=1 1800													
BACKCROUND RANGE-1 1	!SPOT_RANGE=1 900												
BACKGROUND_RANGE=1 10 ! rather use defaults (first 5 degree of rotation)													
UNTRUSTED RECTANGLE= 1800 1950 2100 2150 ! x-min x-max y-min y-max ! repeat													
UNTRUSTED_ELLIPSE= 2	UNTRUSTED_ELLIPSE= 2034 2070 1850 2240 ! x-min x-max y-min y-max ! if needed												
!UNTRUSTED_QUADRILAT	ERAL= x1 y1 x	2 y2 x3 y3	x4 y4	! see do	cumentatior	1							
	•				10 1 1110			-)					
TRUSTED_REGION=0.0 1	.2 ! partially	y use corn	ers of (detector	(0 1.4143)	: use all	pixer	S)					
DETECTOR= PILATUS MI	NIMUM_VALID_P	IXEL_VALUE	=0 OVERL	LOAD= 11	79359 !PIL	ATUS							
!SENSOR_THICKNESS= 0	.32												
X-RAY_WAVELENGTH= 0.	97946 V- 0 172 OV-	0 170 +	o moleo (CODDECT	hoppy if fy		110.01/0	ilabla					
NX- 2463 NY- 2527 Q	X- 0.1/2 Q1-	0.172 ! !	o make (UKKEUT	парру ті ті	alles are	unava	LTADIe					
OSCILLATION RANGE= 0	.2000												
!STARTING_ANGLE= 270	.0000												
DIRECTION_OF_DETECTO	R_X-AXIS=1 0	Θ											
DIRECTION_OF_DETECTO	R_Y-AXIS=0 1	0											

INIT – look at the background



COLSPOT – the spot picker

Monu Hol	QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial														
Menu Hei	þ														
Projects	Frame	XDS.INP	XYCORR	INIT	COLSPOT	IDXREF	DEFPIX	INTEGRATE	CORRECT	tools	statistics	XDSCONV	XSCALE		
			Save Run XDS												
JOB= C	JOB= COLSPOT														
NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_????.cbf DATA_RANGE=1 1800 SPOT_RANGE=1 900 ! BACKGROUND_RANGE=1 10 ! rather use defaults (first 5 degree of rotation) STRONG_PIXEL=4 ! COLSPOT: only use strong reflections (default is 3) MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=3 ! default of 6 is sometimes too high															
DETECT ! SENSO X-RAY_ NX= 24	DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359 !PILATUS !SENSOR_THICKNESS= 0.32 X-RAY_WAVELENGTH= 0.97946 NX= 2463 NY= 2527 QX= 0.172 QY= 0.172 ! to make CORRECT happy if frames are unavailable														
OSCILLA !START DIRECT DIRECT	ATION_R ING_ANG ION_OF_ ION_OF_	ANGE= 0. LE= 270. DETECTOR DETECTOR	2000 0000 _X-AXIS= _Y-AXIS=	100 010											

COLSPOT – the spot picker

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Menu Help



IDXREF – auto-indexing

	QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial												
<u>M</u> enu He <u>l</u>	р												
Projects	Frame	XDS.INP	XYCORR	INIT	COLSPOT	IDXREF	DEFPIX	INTEGRATE	CORRECT	tools	statistics	XDSCONV	XSCALE
						S	ave				Run XDS		
JOB= IDXREF ORGX= 1231.50 ORGY= 1263.50 ! values from frame header; only read by XYCORR, IDXREF DETECTOR_DISTANCE= 189.16000 !read by XYCORR, IDXREF. Negative if detector normal points to crystal. OSCILLATION_RANGE= 0.2000 X-RAY_WAVELENGTH= 0.97946 ! NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_????.cbf ! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing SPOT_RANGE=1 900 SPACE_GROUP_NUMBER= 96 ! 0 if unknown UNIT_CELL_CONSTANTS= 78 78 37 90 90 90 ! put correct values if known INCLUDE_RESOLUTION_RANGE=50 0 ! after CORRECT, insert high resol limit; re-run CORRECT ! EXCLUDE_RESOLUTION_RANGE= 3.93 3.87 !ice-ring at 3.897 Angstrom TRUSTED_REGION=0.0 1.2 ! partially use corners of detector (0 1.4143; use all pixels)													
REFINE ! MINI	(IDXREF MUM_FRA)=CELL B CTION_OF	EAM ORIE _INDEXED	NTATI	ON AXIS S= 0.5	! refine	e POSITI	ON only if	known tha	at hea	der dista	ance inacc	urate
ROTATIO	ROTATION_AXIS=1 0 0 ! Australian Synchrotron, SERCAT ID-22 (?), APS 19-ID (?), ESRF BM30A, SPring-8, SSRF BL INCIDENT_BEAM_DIRECTION=0 0 1 ! only read by IDXREF												
DETECTO NX= 240 DIRECTO DIRECTO	OR= PIL 63 NY= ION_OF_ ION_OF_	ATUS MIN 2527 QX DETECTOR DETECTOR	IMUM_VAL = 0.172 _X-AXIS= _Y-AXIS=	ID_PI QY= 100 010	XEL_VALUE 0.172 ! t	=0 OVERI o make (LOAD= 11 CORRECT	79359 !PII happy if fi	_ATUS rames are	unava	ilable		

First	ge nui	mber	XPARM.XDS								
		Startin	ig phi	Delt	a-phi	1 DIIT 0	2021(spi	indle vector
		×270.	.0000	reb :	2000).999971	0.0)7404	-0.00183		eam vector
space 9	0.9' 5	79460 78.82	215	0.000)711 3215	0.00 37.178)0291 }4 9().000	1.02097 90.000	0 < 90.000	unit cell
group number	36.3	38257 57738	7	9.32 ⁻ 70.532	7419 2730	-69.32 23.30	20709 27367	a b ce	ll vectors	;	
det pane	30.5	59622	-1 2463 p i	.6.002 xels 2	2089 2527	13.86	56352)0	0.172	ai space	el size	
origin 12	231.5	00000	126	53.500	0000	189.16	50004	dista	nce		
	1.0	00000		0.000)000)000)000	0.00)00000)00000	y y z	Detector fast/slow		
Pane	el # 1	0.00	1	00	2463	1)0 0	2527		0 1 0000	

IDXREF – auto-indexing

			c	QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial
<u>M</u> enu He <u>l</u> p			BRAVAIS-	- POSSIBLE SPACE-GROUPS FOR PROTEIN CRYS
Projects Fran	me XDS.INP	XYCORR INI	TYPE	[SPACE GROUP NUMBER, SYMBOL]
	RRAVATC		aP	[1,P1]
	LATTICE	OF FTT	mP	[3, P2] $[4, P2(1)]$
CHAINETER	LATTICE	01 111	mC,mI	[5,C2]
* 44	aP	0.0	0P	[16.P222] $[17.P222(1)]$ $[18.P2(1)2(1)2]$ $[19.P2(1)]$
* 31	aP	0.2	00	$[21 \ C222] \ [20 \ C222(1)]$
* 34	mP mB	1.5	OF	[22,0222] [20,0222(1)]
* 33	mP	2.9	OF	[22, 222]
* 32	oP	3.1	- DI	$\begin{bmatrix} 23, 1222 \end{bmatrix} \begin{bmatrix} 24, 12(1)2(1)2(1) \end{bmatrix}$
* 25	mC	4.5		[75, P4] $[76, P4(1)]$ $[77, P4(2)]$ $[78, P4(3)]$ $[89, P42$
* 23	oC	4.9		[91, P4 (1) 22] [92, P4 (1) 2 (1) 2] [93, P4 (2) 22] [94, P4
* 20	mC	5.1		[95,P4(3)22] [96,P4(3)2(1)2]
* 21	tP mC	6.2	tI	[79,I4] [80,I4(1)] [97,I422] [98,I4(1)22]
39	mC oC	248.0	hP	[143,P3] [144,P3(1)] [145,P3(2)] [149,P312] [150
29	mC	249.9		[152,P3(1)21] [153,P3(2)12] [154,P3(2)21] [168,P
28	mC	250.9		[170, P6(5)] [171, P6(2)] [172, P6(4)] [173, P6(3)]
37	mC	251.4		[178 P6(1)221 [179 P6(5)221 [180 P6(2)221 [181 P
36	oC	252.7	hD	[1/6, 10(1/22)] $[1/3, 10(3/22)]$ $[100, 10(2/22)]$ $[101, 1]$
27	mC	498.8		
19	oI	501.9	CP	[195, P23] [198, P2(1)3] [207, P432] [208, P4(2)32]
26	0F + T	622.5		[213,P4(1)32]
18		025.0	cF	[196,F23] [209,F432] [210,F4(1)32]
2	hR	999.0	cI	[197,I23] [199,I2(1)3] [211,I432] [214,I4(1)32]
3	cP	999.0	3/.2	8.8 /8.8 90.0 90.0
5	cI	999.0	87.2 8	7.1 111.4 50.3 50.3 Range
4	•			start 📃

INTEGRATE – measure the spots!

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds tutorial Menu Help XDS.INP Frame XYCORR COLSPOT DEFPIX XSCALE Projects INIT IDXREF tools statistics XDSCONV Run XDS Save JOB= INTEGRATE NAME_TEMPLATE OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_????.cbf DATA RANGE=1 1800 ! EXCLUDE DATA RANGE= 1000 1100 SPACE GROUP NUMBER=0 ! 0 if unknown UNIT CELL CONSTANTS= 70 70 40 90 90 90 9 put correct values if known **INCLUDE RESOLUTION RANGE=50 0** ! after CORRECT, insert high resol limit; re-run CORRECT !FRIEDEL'S_LAW=FALSE ! This acts only on the CORRECT step REFINE(INTEGRATE) = POSITION BEAM ORIENTATION ! AXIS CELL !NUMBER_OF_PROFILE_GRID_POINTS_ALONG_ALPHA/BETA=13 ! Default is 9 - Increasing may improve data BEAM DIVERGENCE= 0.50204 BEAM DIVERGENCE E.S.D.= 0.05020 !REFLECTING_RANGE= 0.65025 REFLECTING_RANGE_E.S.D.= 0.09289 DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359 !PILATUS X-RAY WAVELENGTH= 0.97946 NX= 2463 NY= 2527 QX= 0.172 QY= 0.172 ! to make CORRECT happy if frames are unavailable OSCILLATION_RANGE= 0.2000 DIRECTION_OF_DETECTOR_X-AXIS=1 0 0 DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0

CORRECT – scale all the "factors"

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds tutorial Menu Help XDS.INP Frame XYCORR INIT COLSPOT IDXREF DEFPIX XSCALE Projects INTEGRATE tools statistics XDSCONV Run XDS Save JOB= CORRECT !NAME_TEMPLATE_OF_DATA_FRAMES=/data/holton/demo/lyso1_189mm_1_????.cbf ! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing DATA RANGE=1 1800 ! EXCLUDE DATA RANGE=1000 1100 SPACE GROUP NUMBER=0 ! 0 if unknown UNIT_CELL_CONSTANTS= 70 70 40 90 90 90 9 put correct values if known INCLUDE_RESOLUTION_RANGE=50 0 ! after CORRECT, insert high resol limit; re-run CORRECT !EXCLUDE_RESOLUTION_RANGE= 3.93 3.87 !ice-ring at 3.897 Angstrom FRIEDEL'S_LAW=FALSE ! This acts only on the CORRECT step **! STRICT ABSORPTION CORRECTION=TRUE** ! REFINE(CORRECT)=CELL BEAM ORIENTATION AXIS POSITION ! Default is: refine everything **FRACTION_OF_POLARIZATION=0.98** ! better value is provided by beamline staff! ! only used by CORRECT POLARIZATION PLANE NORMAL=0 1 0 DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE=0 OVERLOAD= 1179359 !PILATUS SENSOR THICKNESS= 0.32 X-RAY_WAVELENGTH= 0.97946 NX= 2463 NY= 2527 QX= 0.172 QY= 0.172 ! to make CORRECT happy if frames are unavailable OSCILLATION_RANGE= 0.2000 !STARTING ANGLE= 270.0000 DIRECTION_OF_DETECTOR_X-AXIS=1 0 0 DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0



xdsconv – make an "mtz" file

Menu Help

QT5 XDSGUI 2020-12-02 running in /mnt/home1/rapidata3/xds_tutorial

Frame XYCORR COLSPOT IDXREF INTEGRATE XDSCONV Projects XDS.INP INIT DEFPIX CORRECT tools statistics XSCALE run XDSCONV save ! UNIT CELL CONSTANTS= 10 20 30 90 90 90 ! SPACE GROUP NUMBER= 96 ! GENERATE FRACTION OF TEST REFLECTIONS=0.05 INPUT FILE=XDS ASCII.HKL OUTPUT FILE=temp.hkl CCP4 I+F ! or CCP4 I or CCP4 F or SHELX or CNS FRIEDEL'S LAW=FALSE ! store anomalous signal in output file even if weak ! further options see http://xds.mpimf-heidelberg.mpg.de/~kabsch/xds/html doc/xdsconv parameters.html output file name.mtz

Adding noise

1 + 1 = 1.4

$\sigma_{\text{total}}^2 = \sigma_1^2 + \sigma_2^2$

Adding noise $1^2 + 1^2 = 1.4^2$ $3^2 + 1^2 = 3.2^2$ $\sigma_{\text{total}}^2 = \sigma_1^2 + \sigma_2^2$

Adding noise $1^2 + 1^2 = 1.4^2$ $3^2 + 1^2 = 3.2^2$ $10^2 + 1^2 = 10.05^2$



"If you don't have good data, then you must learn statistics."

-James Holton

Sources of error for anomalous differences

- Shutter jitter (rms 0.5 ms)
- Beam flicker (0.15%/sqrt(Hz))
- Attenuation correction (< 2%)
- Radiation damage (1%/MGy)
- Detector calibration (3%)

anomalous signal

$\frac{\Delta F}{F} \approx 1.2 \text{ f"} \sqrt{\frac{\text{\# sites}}{MW (Da)}}$

Crick, F. H. C. & Magdoff, B. S. (1956) *Acta Crystallogr.* **9**, 901-908. Hendrickson, W. A. & Teeter, M. M. (1981) *Nature* **290**, 107-113.

🕙 required number of crystals calculator - Mozilla Firefox												
<u>File E</u> dit <u>V</u> iew Hi <u>s</u> tory <u>B</u> ookmarks <u>T</u> ools <u>H</u> elp												
🕜 🕞 🗸 🏠 📋 http://bl831.als.lbl.gov/xtalsize.html 🗘 🔹 👿 🗸 Wikipedia (en)												
required number of crystals calculator												
Required crystal number or size calculator												
n / 20. * 6 •	* \ ATU	$* \sqrt{2} / \sqrt{2} $	rtalaiza ³ / (raga ³ 1	52)								
nxtals — <idl> / 20 * iNi</idl>	H IVI W	VM (exp(-0.5 Direso))	XLAISILE) (TESO - T.)))								
Enter values:								=				
experiment goal =	subtle o	lifferences (MAD/SAD) 🔽										
number of sites =	1	in asymmetric unit										
fpp =	4	electrons	Bijvoet ratio =	1.75	%							
molecular weight =	30	kDa in asymmetric unit										
resolution =	3.4	Ang	signal to noise =	81	at this resolut	ion						
reso on snapshot =	2.4	Ang	\rightarrow Wilson B =	35] Ang ²							
background level =	100	ADU/pixel	multiplicity =	7.3								
spot size =	5	pixels										
detector type =	ADSC	Q210/315r (hwbin) 🛛 🛛 🔽										
solvent content =	50	%										
xtal size _{beam} =	20	microns										
xtal size _{vert} =	20	microns	beam size _{vert} =	100	microns							
xtal size _{spindle} =	20	microns	beam size _{spindle} =	100	microns							
Calculate n_xtals	Calculate n_xtals ↓ Calculate size ↑											
$n_{xtals} =$	1.4	xtals you will need to merge	$\leftarrow < I_{DL} >$	11000	photons/hkl							
Dopo							1	×				
Done							Sec. 1	J .::				

Holton & Frankel (2010) Acta D 66 393-408.

Re-indexing cheat sheet

Space group	Re-indexing
$P4$, ($P4_1$, $P4_3$), $P4_2$, $I4$, $I4_1$	$hkl \rightarrow kh\overline{l}$
$P3, (P3_1, P3_2)$	$hkl \rightarrow \overline{hkl}$
	or $hkl \rightarrow kh$
	or $hkl \rightarrow \overline{kh}$
<i>R</i> 3	$hkl \rightarrow kh\overline{l}$
$P321, (P3_121, P3_221)$	$hkl \rightarrow \overline{hkl}$
$P312, (P3_112, P3_212)$	$hkl \rightarrow \overline{hkl}$
$P6, (P6_1, P6_5), (P6_2, P6_4), P6_3$	$hkl \rightarrow kh\overline{l}$
$P23, P2_13, (I23, I2_13), F23$	$hkl \rightarrow k\overline{h}l$

Dauter, Z. (1999). "Data-collection strategies." Acta Cryst. D 55(10): 1703-1717.

Zero-dose extrapolation (ZDE)



Example of noisy data points (marked by '+') fitted by a linear (green), a quadratic (blue) and an exponential function (purple). Near 1/4 and near 3/4 of the range, the values of the functions used for fitting coincide.

radiation aspects of ю О (2006). "Some ത analysis Crvst . ک cta **Diederichs**, quantitativ damage

xscale – final stats

					QT5 XDSG	UI 2020-12-0	2 runnin	ng in /mnt/hon	ne1/rapidata	3/xds_tutoria	I				
He <u>l</u> p	He <u>l</u> p														
cts	Frame	XDS.INP	XYCORR	INIT COL	SPOT IDXREF	DEFPIX	INTEC	GRATE CO	RRECT to	ols statis	tics XDSC	CONV	XSCALE	SHELX	
save								run xscale	9			show XSC/			
BSET SOLU LIMI	OF IN TION T	NTENSITY NUMBE OBSERVED	DATA WITH R OF REFL UNIQUE	H SIGNAL/M LECTIONS POSSIBLM	NOISE >= -3 COMPLETE E OF DA	.0 AS FUN NESS R-FA TA obse	NCTION ACTOR erved	OF RESOL R-FACTOF expected	UTION COMPARE	D I/SIGM	A R-mea	as	CC(1/2)	Anomal Corr	
4.	82	15416	1089	1093	L 99.3	3%	1.1%	1.8%	5 1541	.6 145.6	7 1	.2%	100.0*	89*	
з.	41	24671	1848	1955	5 94.	5%	1.4%	1.9%	5 2466	6 140.2	6 1	.5%	100.0*	69*	
2.	78	36341	2537	2537	7 100.	9%	1.6%	1.9%	5 3634	1 132.8	4 1	.7%	100.0*	46*	
2.	41	37752	3013	3014	4 100.	9%	2.1%	2.1%	5 3775	2 106.6	3 2	.2%	100.0*	41*	
2.	16	46702	3405	3405	5 100.	9%	2.6%	2.4%	5 4670	96.9	0 2	.7%	100.0*	36*	
1.	97	51923	3756	3756	5 100.	9%	3.3%	2.9%	5192	23 78.7	9 3	.4%	100.0*	19*	
1.	82	51323	4111	4113	l 100.	9%	4.7%	4.0%	5132	23 54.2	6 4	.9%	99.9*	14*	
1.	71	57891	4362	4362	2 100.	9%	7.2%	6.3%	5789	1 38.4	5 7	.5%	99.9*	9	
1.	61	64156	4680	4680	9 100.	9%	9.8%	9.1%	6415	6 28.1	7 10	.2%	99.8*	3	
1.	53	68501	4943	4943	B 100.	9% 1	L4.3%	14.1%	6850	1 19.3	1 14	.9%	99.7*	3	
1.	45	64913	5219	5219	9 100.	9% 2	20.3%	20.4%	6491	.3 13.2	0 21	.2%	99.3*	0	
1.	39	72865	5446	5447	7 100.	9% 3	32.4%	33.9%	5 7286	5 8.6	3 33	.7%	98.5*	- 5	
1.	34	77152	5660	5660	9 100.)% 2	17.7%	50.5%	5 7715	52 5.9	9 49	.6%	97.3*	-1	
1.	29	74358	5893	5893	3 100.	3 % 6	56.2%	70.6%	5 7435	68 4.1	3 69	.0%	94.9*	- 3	
1.	25	78139	6102	6103	3 100.	9% <u>9</u> %	97.4%	105.1%	5 7813	39 2.8	2 101	.4%	88.6*	-1	
1.	21	83395	6304	6304	4 100.	9% 13	31.6%	143.4%	5 8339	5 2.0	7 136	.8%	82.6*	- 4	
1.	17	82112	6550	6553	l 100.	9% 17	72.1%	189.4%	5 8211	.2 1.4	5 179	.4%	70.6*	- 2	
1.	14	57381	6701	6703	l 100.	0% 2 3	32.2%	256.3%	5738	81 0.8	0 247	.1%	41.3*	- 5	
1.	11	41788	6847	6918	B 99.	3% 3 6	97.2%	341.0%	5 416 8	9 0.4	6 335	.7%	19.2*	1	
1.	08	26251	6266	7083	l 88.	5% 45	56.8%	513.1%	5 2559	0.2	2 518	.3%	7.1	Θ	
tot	al	1113030	94732	95733	1 99.0	9%	2.9%	3.2%	5 111226	8 26.8	5 3	.0%	100.0*	2	
			2										-		

XDS: CORRECT.LP or XSCALE.LP

OMPARED	I/SIGMA	R-meas	CC (1/2)	Anomal	SigAno	
				Corr		
3018	33.77	2.3%	99.9*	21*	1.012	
4585	22.56	3.6 %	99.8*	9	0.914	
5327	19.99	4.0 %	99.7*	9	0.859	
6094	12.27	6.8 %	99.3*	-1	0.784	
7068	6.01	14.2 %	97.8*	-2	0.799	
8185	3.10	29.4 %	88.8*	-4	0.776	
8981	1.90	48.8 %	75.9*	2	0.765	
5991	1.14	87.3%	53.5*	-2	0.722	
2520	0.59	170.4%	21.9*	4	0.693	
51769	8.97	9.5 %	99.5*	2	0.804	
XDS: CORRECT.LP or XSCALE.LP

CORRECTION PARAMETERS FOR THE STANDARD ERROR OF REFLECTION I

The variance vO(I) of the intensity I obtained from counting st replaced by $v(I)=a^*(vO(I)+b^*I^2)$. The model parameters a, b are minimize the discrepancies between v(I) and the variance estima sample statistics of symmetry related reflections. This model i an asymptotic limit ISa=1/SQRT(a*b) for the highest I/Sigma(I) experimental setup can produce (Diederichs (2010) Acta Cryst D6

CCP4: aimless log

\$TABLE: Analysis against resolution, XDSdataset: \$GRAPHS:I/sigma, Mean Mn(I)/sd(Mn(I)):0|0.216023x0|137.14:2,13,14: :Rmerge, Rfull, Rmeas, Rpim v Resolution:0|0.216023x0|1.70834:2,4,5,6,7: :Average I, RMSdeviation and Sd:0|0.216023x0|1650.8:2,10,11,12: :Fractional bias:0|0.216023x0|0:2,15:

\$\$

Ν	1/d^2	Dmid	Rmrg	Rfull	Rcum	Rmeas	Rpim	Nmeas	AvI	RMSdev	sd	I/R ^M S	Mn(I/sd)	Frd
1	0.0064	12.55	0.020	0.020	0.020	0.021	0.006	13115	1651	57	42	29.2	137.1	
2	0.0191	7.24	0.027	0.027	0.024	0.028	0.008	24753	1171	47	42	25.0	105.2).
3	0.0318	5.61	0.038	0.038	0.029	0.040	0.012	32197	857	46	43	18.4	79.6	
4	0.0445	4.74	0.034	0.034	0.031	0.035	0.010	37743	<u>1212</u>	57	53	21.4	91.2	
5	0.0572	4.18	0.036	0.036	0.032	0.038	0.011	42642	1181	59	57	19.9	83.8	
6	0.0699	3.78	0.049	0.049	0.036	0.052	0.015	47224	883	59	57	15.1	65.1	
7	0.0826	3.48	0.065	0.065	0.040	0.068	0.020	51052	685	59	58	11.7	50.9	
8	0.0953	3.24	0.096	0.096	0.045	0.100	0.029	54636	448	56	56	8.0	35.0	•
9	0.1080	3.04	0.151	0.151	0.050	0.158	0.046	58072	268	53	53	5.1	22.7	
10	0.1207	2.88	0.229	0.229	0.056	0.240	0.070	60731	171	51	51	3.3	15.4	
11	0.1334	2.74	0.314	0.314	0.063	0.329	0.097	63807	125	51	51	2.4	11.3	
12	0.1461	2.62	0.406	0.406	0.070	0.425	0.125	66241	98	51	52	1.9	8.7	
13	0.1588	2.51	0.537	0.537	0.078	0.562	0.166	68272	76	53	53	1.4	6.5	

CCP4: aimless log

\$TABLE: Correlations CC(1/2) within dataset, XDSdataset: \$GRAPHS: Anom & Imean CCs v resolution:0|0.216023x0|1:2,4,7: : RMS correlation ratio :0|0.216023x0|2.20344:2,6: \$\$

Ρ₽							
Ν	1/d^2	Dmid	CCanom	Nanom	RCRanom	CC1/2	NImean
1	0.0064	12.55	0.659	499	2.203	1.000	669
2	0.0191	7.24	0.550	975	1.853	1.000	1155
3	0.0318	5.61	0.527	1295	1.798	1.000	1479
16	0.1970	2.25	0.037	2123	1.038	0.711	2275
17	0.2097	2.18	0.043	1682	1.044 (0.460	1877

Resolution cutoff?



Average outer-shell R_{merge}

Expected R_{merge} as $I_{obs} \rightarrow 0$

$R_{merge} = \frac{\sum \left| I_{obs} - \langle I \rangle \right|}{\sum I_{obs}}$

Optimum resolution cutoff is:

- Too optimistic: add nothing but noise
- Too pessimistic: series-termination error
- Happy medium?
- Simulate:
 - Random atoms, compute F²
 - Add Gaussian noise, RMS = 1
 - Truncate
 - Subtract "right" map, RMS difference

Optimal resolution cutoff



Optimal resolution cutoff



Optimal resolution cutoff



Wilson Plot



∞ 2.2 1.6 1.3 1.1 1.0 0.9 0.85 0.8 0.75 0.7 resolution (Å)

Optimum resolution cutoff is:

0.0Å







scattering x-ray beam

sample









scattering from a structure

sample detector direct beam

formersed Fourier Transform

no phase



sidattes en El droi en al same forme

colored by phase

sample



scattering from a lattice

colored by phase

sample



scattering from a lattice

colored by phase

sample

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scattering from a lattice

colored by phase

sample





scattering from a crystal structure

colored by phase

sample



Major Phasing techniques

- Molecular Replacement
- Multiple Isomorphous Replacement
- Multiwavelength Anomalous Diffraction
- Single-wavelength Anomalous Diffraction

inverse Fourier Transform

no phase



inverse Fourier Transform

no phase



Major Phasing techniques

- Molecular Replacement
- Multiple Isomorphous Replacement
- Multiwavelength Anomalous Diffraction
- Single-wavelength Anomalous Diffraction









