

# Data Collection Strategy

## COSMO for GADDS and SMART Data Collection

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**Cosmo for GADDs**

Point to File/Load Configuration. Find cosmo\_5.ini (normally in F:\frames\ ) for the 5 cm detector distance.

Point to File/Import Crystal Data import your file

Point to Refine Strategy and let the program refine a few seconds

Source	HVPC	ZTheta	Omega	Phi	Chi	Axis	Width	#Frames	Sweep
Custom	5.00	-35.00	-35.00	+0.00	+54.70	Omega	-0.50	360	180.00
Custom	5.00	-35.00	-35.00	+90.00	+54.70	Omega	-0.50	360	180.00
Custom	5.00	-35.00	-35.00	+180.00	+54.70	Omega	-0.50	360	180.00
Custom	5.00	-90.00	+270.00	+0.00	+54.70	Omega	-0.50	360	180.00
Custom	5.00	-90.00	+270.00	+90.00	+54.70	Omega	-0.50	360	180.00
Custom	5.00	-90.00	+270.00	+180.00	+54.70	Omega	-0.50	360	180.00
Custom	5.00	-90.00	+270.00	+270.00	+54.70	Omega	-0.50	360	180.00
Intern	5.00	-85.00	-165.00	+359.50	+54.74	Phi	-0.50	719	359.50
Intern	5.00	-25.00	-85.00	+359.50	+54.74	Phi	-0.50	719	359.50
Intern	5.00	-40.00	-160.00	+174.13	+54.74	Phi	-0.50	348	174.00
Intern	5.00	-70.00	-110.00	-0.50	+54.74	Phi	-0.50	213	106.50
Intern	5.00	-20.00	-120.00	+359.50	+54.74	Phi	-0.50	719	359.50
Intern	5.00	-10.00	-75.00	+359.50	+54.74	Phi	-0.50	719	359.50
Intern	5.00	-85.00	-115.00	-0.50	+54.74	Phi	-0.50	124	62.00
Intern	5.00	-85.00	-110.00	-0.50	+54.74	Phi	-0.50	584	292.00
Intern	5.00	-80.00	-180.00	+44.93	+54.74	Phi	-0.50	90	45.00
Intern	5.00	-80.00	-155.00	+213.45	+54.74	Phi	-0.50	427	213.50
Intern	5.00	-80.00	-130.00	+73.02	+54.74	Phi	-0.50	146	73.00
Intern	5.00	-80.00	-120.00	+359.50	+54.74	Phi	-0.50	719	359.50
Intern	5.00	-80.00	-110.00	+359.50	+54.74	Phi	-0.50	719	359.50
Intern	5.00	-80.00	-105.00	+95.49	+54.74	Phi	-0.50	191	95.50
Intern	5.00	-80.00	-95.00	+202.22	+54.74	Phi	-0.50	404	202.00
Intern	5.00	-80.00	-85.00	+213.45	+54.74	Phi	-0.50	427	213.50
Intern	5.00	-75.00	-150.00	-0.50	+54.74	Phi	-0.50	292	146.00
Intern	5.00	-70.00	-140.00	+331.41	+54.74	Phi	-0.50	663	331.50
Intern	5.00	-70.00	-130.00	+254.01	+54.74	Phi	-0.50	528	254.00
Intern	5.00	-90.00	-105.00	+359.50	+54.74	Phi	-0.50	719	359.50
Intern	5.00	-70.00	-100.00	-0.50	+54.74	Phi	-0.50	506	253.00
Intern	5.00	-70.00	-80.00	-0.50	+54.74	Phi	-0.50	67	33.50
Intern	5.00	-70.00	-75.00	+359.50	+54.74	Phi	-0.50	719	359.50

Point and hold (left mouse button)

Refine Strategy and choose the sort runs option let the program sort the runs.

Point to View/Detailed Strategy. The black is the permanent strategy from cosmo\_5.ini. The blue is the extra frames from cosmo. Select all of the blue and then right click. Disable the

	Current	Target	Priority
Completeness [%]:	96.47	100.00	100
Redundancy:	2.54	4.00	20
Time [h]:	7.00	24.00	5
Strategy:	Custom		

Sort Runs for Completeness

sets. Return to main menu screen. Take note of the Completeness. In this case the default

Bijvoet Pairs:	merged
Laue Class:	-1
Lattice Type:	P

strategy is 96% complete without any new data sets. This is for a triclinic data set in the space group P-1. I would like to collect ALL of the data for a P1

Bijvoet Pairs:	not merged
Laue Class:	-1
Lattice Type:	P

space group. Therefore change the Bijvoet Pairs to not-merged by pointing to merged and

	Current	Target	Priority
Completeness [%]:	78.06	100.00	100
Redundancy:	1.57	4.00	20
Time [h]:	7.00	24.00	5
Strategy:	Custom		

Sort Runs for Completeness

left clicking. Now check the Completeness.

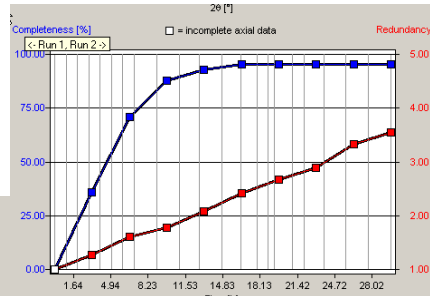
We are not at 78% which is unacceptable (should be near 90%). Run the refine strategy by pointing at the sort runs button and left clicking. Let the program run until at least 90% completeness is seen (higher is better). Note the

results. After run 12 the blue line (% completeness line) levels off. We can stop the data collection after the 12 set of frames and still have a complete data set. Point to View/Detailed Strategy and select all frame sets after # 12, right click them and disable them.

Now pick all the remaining blue sets,

	Current	Target	Priority
Completeness [%]:	95.23	100.00	100
Redundancy:	2.42	4.00	20
Time [h]:	16.45	24.00	5
Strategy:	Custom		

Sort Runs for Completeness



right click them and make them permanent. Return to main menu and note the completeness (in this case ~95%) with ok redundancy 2.4. Point to File/Export strategy and write a text file with the results.

In FRAMBO (or GADDS or SMART) point to COLLECT/SCANS EDITRUNS highlight all of the frame sets and delete them. Point to READ and import the text file you made with COSMO. Edit this file. Remember to always place a space between numbers. (e.g. when editing line 09 place a space between -90.000 and -170.000).

Run#	Frame#	2-Theta	Omega	Phi	Chi	Axis	Width	#Frames	Time
01	001	-35.000	-35.000	0.000	54.700	2	-0.500	360	10.00
02	001	-35.000	-35.000	90.000	54.700	2	-0.500	360	10.00
03	001	-35.000	-35.000	180.000	54.700	2	-0.500	360	10.00
04	001	-90.000	270.000	0.000	54.700	2	-0.500	360	10.00
05	001	-90.000	270.000	90.000	54.700	2	-0.500	360	10.00
06	001	-90.000	270.000	180.000	54.700	2	-0.500	360	10.00
07	001	-90.000	270.000	270.000	54.700	2	-0.500	360	10.00
08	001	-80.000	-95.000	359.500	54.740	3	-0.500	719	10.00
09	001	-90.000	-170.000	359.500	54.740	3	-0.500	719	10.00
10	001	-65.000	-70.000	320.180	54.740	3	-0.500	640	10.00
11	001	-70.000	-130.000	359.500	54.740	3	-0.500	719	10.00
12	001	-50.000	-55.000	-0.500	54.740	3	-0.500	607	10.00

Be sure to use the CURSOR KEYS to move between number NOT THE MOUSE

08	001	-80.000	-95.000	359.500	54.740	3	-0.500	719	10.00
09	001	-90.000	-170.000	359.500	54.740	3	-0.500	719	20.00
10	001	-65.000	-70.000	320.180	54.740	3	-0.500	640	10.00
11	001	-70.000	-130.000	359.500	54.740	3	-0.500	719	10.00

Change the time to fit your data collection etc.

Start the data collection normally.