

Unattended Data Collection (UDC) User Training

March 2023

UDC: Background

- UDC is a ship and forget collection system. It might not handle all cases (yet) but should cope well with the majority.
- UDC collection parameters are automatically set based on end use case. No need to worry about technicalities of the beamline.
- Aim is for complete, well-measured datasets that do not exhibit major radiation damage. Autoprocessed data should be usable without reprocessing and combining datasets should be trivial.
- The workflow is efficient & reliable. Well over 100,000 samples collected so far.
- Post collection samples can be moved to a standard remote session for any further collection desired.

UDC: What is in scope

When to use UDC	When not to use UDC
Single crystals (>20 μ m)	Split crystals, multiple lattices, microcrystals
Projects requiring data collections from many crystals <ul style="list-style-type: none">• searching for highest resolution native• ligand binding studies Rapid feedback on a well characterised system from a small number of new crystals	Projects requiring manual input e.g. <ul style="list-style-type: none">• Selecting best region from a crystal with pathologies• Line or wedged scans• Fluorescence scans
Standard SAD phasing experiments <ul style="list-style-type: none">• Try this first if you have sufficient crystals	Phasing from limited number of crystals Complex multi-crystal phasing experiments
Energy range: 7-18KeV	Energies outside this range are supported in remote access

<https://www.diamond.ac.uk/Instruments/Mx/I03/I03-Manual/Unattended-Data-Collections.html>

UDC: Experiment Kinds

Recipe	Protocol	Samples/hr (without screening)	Samples/hr (with screening)
Native	Prioritises completeness/multiplicity and collects 2 x 360° sweeps, 1st at chi=0 and 2nd at chi=30	20	12
Ligand	Prioritises speed of data collection and collects a single sweep, 360° dataset	30	15
Phasing	Two 360° sweeps are collected using different chi/phi values at your chosen energy, using a lower transmission to maximise anomalous multiplicity and completeness.	20	12
Stepped	Prioritises resolution and conducts a stepped transmission scan	10	-

<https://www.diamond.ac.uk/Instruments/Mx/I03/I03-Manual/Unattended-Data-Collections/Experiment-Types.html>

UDC: Resolution & Screening

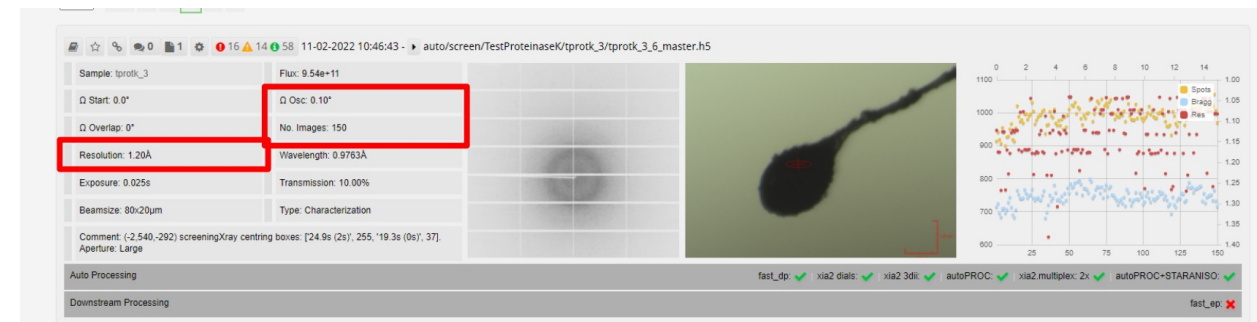
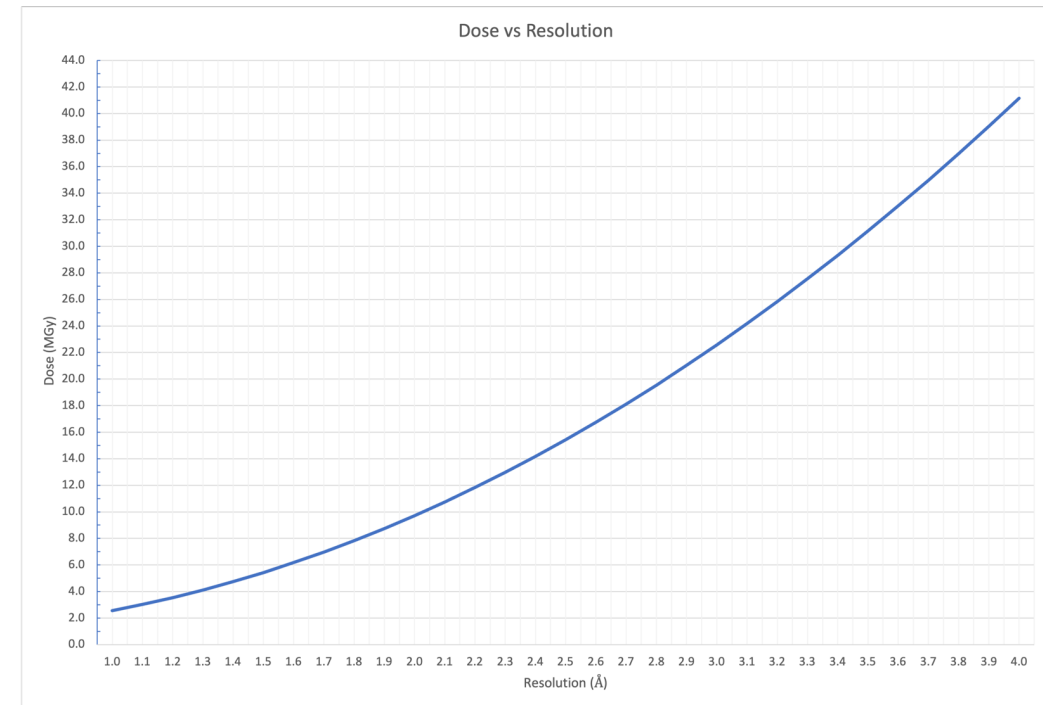
UDC will assign the dose to be used for collection based on the sample resolution. Either:

- User chosen
- Determined via screening

Screening methodology

- 15° wedge collection
- High resolution detector edge, low resolution dose
 - Handles both strong and weak samples
- If Fast_dp fails, move on and return later if other pipelines integrate successfully

Resolution = processing result + padding (0.5Å)



UDC: Screening Modes

Screening takes the same time as collection. Screening modes allow more efficient use of this.

Better than

User defines 'minimum resolution'

Sample is loaded and screened

If screening result is better than minimum resolution, then sample is collected

Collect best 'n'

User defines equivalent samples via 'sample group'
User defines 'n'

Sample group is shipment contained

Every sample in the group is loaded and screened

At the end of screening, the best 'n' samples are reloaded and collected

UDC: Process

Simplified workflow



Beamline: **i04** Last update: 2020-12-14 17:20:49 Force update Baton holder: UDC Visit: mx20147-17 UAS: ISPyB:

Progress	Proposal	Location	Reg. Container	I04 Time	Time Remaining	Samples Approved	Shipment	Tag	Arrived / Loaded	Possible Beamlines	
▼ i04 (loaded) (15 Items)											
1	0/16	mx24447-48	i04 (16)	DLS-406	01:04:00	01:04:00	✓	MANC-091220	5a	2020-12-14 13:22:15	i03,i04
2	0/16	mx24447-48	i04 (17)	DLS-400	00:56:00	00:56:00	✓	MANC-091220	5a	2020-12-14 13:22:54	i03,i04
3	0/16	mx24447-48	i04 (18)	DLS-0030	01:00:32	01:00:32	✓	MANC-091220	5a	2020-12-14 13:23:22	i03,i04
4	0/16	mx24447-48	i04 (19)	DLS-0031	01:03:08	01:03:08	✓	MANC-091220	5a	2020-12-14 13:23:48	i03,i04
5	0/16	mx24447-48	i04 (20)	DLS-0032	01:09:12	01:09:12	✓	MANC-091220	5a	2020-12-14 13:24:15	i03,i04
6	0/16	mx24447-48	i04 (21)	DLS-0033	01:00:32	01:00:32	✓	MANC-091220	5a	2020-12-14 13:24:38	i03,i04
7	0/16	mx24447-48	i04 (22)	DLS-0035	00:56:00	00:56:00	✓	MANC-091220	5a	2020-12-14 13:24:59	i03,i04
8	0/16	mx24447-48	i04 (23)	DLS-401	01:00:32	01:00:32	✓	MANC-091220	5b	2020-12-14 13:25:36	i03,i04
9	0/16	mx24447-48	i04 (24)	DLS-402	01:03:08	01:03:08	✓	MANC-091220	5b	2020-12-14 13:26:09	i03,i04
10	0/16	mx19844-63	i04 (25)	CPS-4371	01:04:39	01:04:39	✓	YK_dewar	11a	2020-12-14 13:30:31	i03,i04
11	0/16		i04 (26)		00:55:40	00:55:40	✓	2020-12-11_DLS_2	6f	2020-12-14 13:31:20	i03,i04
12	0/16		i04 (27)		00:53:15	00:53:15	✓	2020-12-11_DLS_2	6f	2020-12-14 13:31:52	i03,i04
13	0/16		i04 (28)		00:54:59	00:54:59	✓	2020-12-11_DLS_2	6f	2020-12-14 13:32:15	i03,i04
14	0/16		i04 (29)		00:54:24	00:54:24	✓	2020-12-11_DLS_2	6f	2020-12-14 13:32:38	i03,i04
15	0/16		i04 (30)		00:50:16	00:50:16	✓	2020-12-11_DLS_2	6f	2020-12-14 13:33:01	i03,i04
0/240					14:46:17	14:46:17					
▼ dewar store (36 Items)											
16	0/16	mx19844	tray-4e	CPS-5376	00:54:24	00:54:24	✓	DDU_Dec	4e	2020-12-09 15:10:41	i03,i04,i04-1
17	0/16	mx19844	tray-4e	CPS-5377	00:56:20	00:56:20	✓	DDU_Dec	4e	2020-12-09 15:10:41	i03,i04
18	0/8	mx19844	tray-4e	DUN-0001	00:27:12	00:27:12	✓	DDU_Dec	4e	2020-12-09 15:10:41	i03,i04,i04-1
19	0/8	mx19844	tray-4e	DLS-247	00:27:28	00:27:28	✓	DDU_Dec	4e	2020-12-09 15:10:41	i03,i04
20	0/16	mx25402	tray-10d	CXF-0002	00:52:32	00:52:32	✓	09122020_mx25402_automated	10d	2020-12-10 10:29:34	i03,i04,i04-1
21	0/14	mx25402	tray-10d	CXF-0004	00:45:58	00:45:58	✓	09122020_mx25402_automated	10d	2020-12-10 10:29:34	i03,i04,i04-1
22	0/16	mx25402	tray-10d	MH-005	00:52:32	00:52:32	✓	09122020_mx25402_automated	10d	2020-12-10 10:29:34	i03,i04,i04-1
23	0/16	mx25402	tray-10d	MH-007	00:42:41	00:42:41	✓	09122020_mx25402_automated	10d	2020-12-10 10:29:34	i03,i04,i04-1
237/1389					76:14:25	63:52:10					

