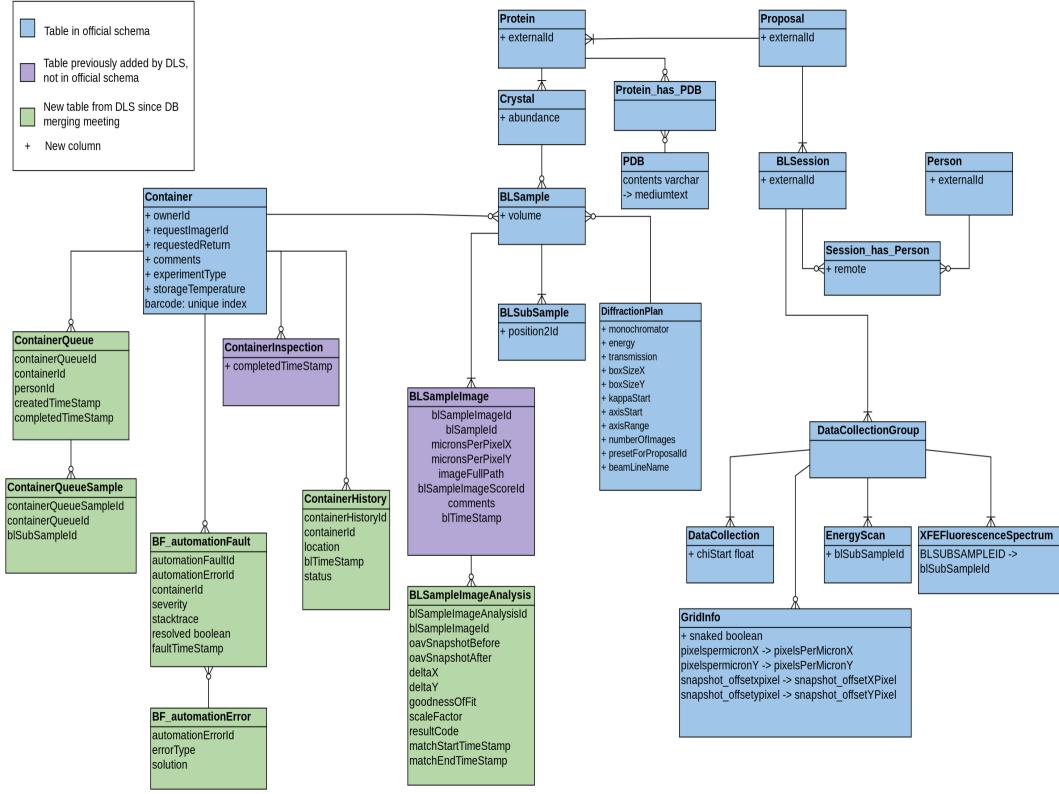
## Diamond ISPyB Schema Changes





## Crystal Imaging – New Columns

- DiffractionPlan (11 cols)
- Container (6 cols)
- ContainerInspection (1 col)



## Crystal Imaging - DiffractionPlan

ADD monochromator varchar(8) COMMENT 'DMM or DCM',

ADD energy float COMMENT 'eV',

ADD transmission float COMMENT 'Decimal fraction in range [0,1]',

ADD boxSizeX float COMMENT 'microns'.

ADD boxSizeY float COMMENT 'microns',

ADD kappaStart float COMMENT 'degrees',

ADD axisStart float COMMENT 'degrees',

ADD axisRange float COMMENT 'degrees',

ADD numberOfImages mediumint COMMENT 'The number of images requested',

ADD **presetForProposalId** int(10) unsigned COMMENT 'Indicates this plan is available to all sessions on given proposal',

ADD **beamLineName** varchar(45) COMMENT 'Indicates this plan is available to all sessions on given beamline',

ADD CONSTRAINT DiffractionPlan\_ibfk1 FOREIGN KEY (presetForProposalId) REFERENCES Proposal (proposalId)



## Crystal Imaging - Container

ADD ownerld int(10) unsigned NULL DEFAULT NULL,

ADD CONSTRAINT Container\_ibfk5 FOREIGN KEY (ownerld), REFERENCES Person (personld)

ADD requestedImagerId int(11) unsigned,

ADD CONSTRAINT Container\_ibfk7 FOREIGN KEY (requestedImagerId) REFERENCES Imager (imagerId),

ADD **requestedReturn** boolean DEFAULT False COMMENT 'True for requesting return, False means container will be disposed',

ADD comments varchar(255),

ADD **experimentType** varchar(20),

ADD **storageTemperature** float



# Crystal Imaging - ContainerInspection

```
`containerInspectionId` int(11) unsigned NOT NULL AUTO_INCREMENT,
```

- `containerId` int(11) unsigned NOT NULL,
- `inspectionTypeId` int(11) unsigned NOT NULL,
- `imagerId` int(11) unsigned DEFAULT NULL,
- `temperature` float DEFAULT NULL,
- `blTimeStamp` datetime DEFAULT NULL,
- `scheduleComponentid` int(11) unsigned DEFAULT NULL,
- `state` varchar(20) DEFAULT NULL,
- `priority` smallint(6) DEFAULT NULL,
- `manual` tinyint(1) DEFAULT NULL,
- `scheduledTimeStamp` datetime DEFAULT NULL,
- `completedTimeStamp` datetime DEFAULT NULL -- NEW column



## Crystal Imaging – Drop Images

- Table : BLSampleImage (not new)
- Table: BLSampleImageAnalysis (new)
- Table: BLSampleImageMeasurement (not live)

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## BLSampleImage (not new)

- `blSampleImageId` int(11) unsigned NOT NULL AUTO\_INCREMENT,
- `blSampleId` int(11) unsigned NOT NULL,
- `micronsPerPixelX` float DEFAULT NULL,
- `micronsPerPixelY` float DEFAULT NULL,
- `imageFullPath` varchar(255) DEFAULT NULL,
- `blSampleImageScoreId` int(11) DEFAULT NULL,
- `comments` varchar(255) DEFAULT NULL,
- `blTimeStamp` datetime DEFAULT NULL,
- `containerInspectionId` int(11) unsigned DEFAULT NULL,
- `modifiedTimeStamp` datetime DEFAULT NULL



## BLSampleImageAnalysis

```
`blSampleImageAnalysisId` int(11) unsigned NOT NULL AUTO_INCREMENT,
```



<sup>`</sup>blSampleImageId` int(11) unsigned DEFAULT NULL,

<sup>`</sup>oavSnapshotBefore` varchar(255) DEFAULT NULL,

<sup>`</sup>oavSnapshotAfter` varchar(255) DEFAULT NULL,

<sup>`</sup>deltaX` int(11) DEFAULT NULL,

<sup>`</sup>deltaY` int(11) DEFAULT NULL,

<sup>`</sup>goodnessOfFit` float DEFAULT NULL,

<sup>`</sup>scaleFactor` float DEFAULT NULL,

<sup>`</sup>resultCode` varchar(15) DEFAULT NULL,

<sup>`</sup>matchStartTimeStamp` timestamp NULL DEFAULT CURRENT\_TIMESTAMP,

<sup>`</sup>matchEndTimeStamp` timestamp NULL DEFAULT NULL

## Crystal Imaging – Container Tables

- Table : ContainerHistory (new)
- Table : ContainerQueue (new)
- Table : ContainerQueueSample (new)



## ContainerHistory

`containerHistoryId` int(11) unsigned NOT NULL AUTO\_INCREMENT,

`containerId` int(10) unsigned DEFAULT NULL,

'location' varchar(45) DEFAULT NULL,

`blTimeStamp` timestamp NOT NULL DEFAULT CURRENT\_TIMESTAMP,

`status` varchar(45) DEFAULT NULL,



## ContainerQueue

`containerQueueld` int(11) unsigned NOT NULL AUTO\_INCREMENT,

`containerId` int(10) unsigned DEFAULT NULL,

'personId' int(10) unsigned DEFAULT NULL,

`createdTimeStamp` timestamp NOT NULL DEFAULT CURRENT\_TIMESTAMP,

`completedTimeStamp` timestamp NULL DEFAULT NULL



## ContainerQueueSample

`containerQueueSampleId` int(11) unsigned NOT NULL AUTO\_INCREMENT,

`containerQueueld` int(11) unsigned DEFAULT NULL,

`blSubSampleId` int(11) unsigned DEFAULT NULL



#### **Automation Fault Tables**

Table : BF\_automationFault (new)

Table : BF\_automationError (new)



### BF\_automationFault

`automationFaultId` int(10) unsigned NOT NULL AUTO\_INCREMENT,

`automationErrorld` int(10) unsigned DEFAULT NULL,

`containerId` int(10) unsigned DEFAULT NULL,

`severity` enum('1','2','3') DEFAULT NULL,

`stacktrace` text,

`resolved` tinyint(1) DEFAULT NULL,

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`faultTimeStamp` timestamp NOT NULL DEFAULT CURRENT TIMESTAMP



## BF\_automationError

`automationErrorld` int(10) unsigned NOT NULL AUTO\_INCREMENT,

`errorType` varchar(40) NOT NULL,

`solution` text



#### Misc columns

- Crystal: abundance float
- BLSample: volume float
- BLSubSample: position2Id int(11) unsigned
- PDB: contents varchar → mediumtext; (approx 16MB)
- Session\_has\_Person: remote boolean
- DataCollection: chiStart float

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EnergyScan: blSubSampleId int(11) unsigned

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GridInfo: snaked boolean



#### GUID columns

- **Proposal**: externalld binary(16)
- **BLSession**: externalld binary(16)
- Person : externalld binary(16)
- Protein : externalld binary(16)



#### GUID columns – hex function

[ispyb]> select **hex(**externalId) from Person where personId = 52828;

```
+----+
```

| hex(externalId)

+----+

+----+

1 row in set (0.00 sec)



## Proposed: ContainerType

containerTypeId int(11) unsigned auto increment NOT NULL PRIMARY KEY, `name` varchar(45) NOT NULL COMMENT 'Short name', fullName varchar(45) NOT NULL COMMENT 'Full name including manufacturer', **capacity** smallint unsigned COMMENT 'Total n.o. drops', wellsPerRow tinyint unsigned, dropsPerWellX tinyint unsigned, dropsPerWellY tinyint unsigned, dropHeight float COMMENT '0.0 - 1.0 percentage of well height', **dropWidth** float COMMENT '0.0 - 1.0 percentage of well width', **dropOffsetX** float COMMENT '0.0 - 1.0 percentage offset from top-left corner of well', dropOffsetY float COMMENT '0.0 - 1.0 percentage offset from top-left corner of well', wellDrop smallint COMMENT 'Number of the drop which is the well (i.e. reservoir)'



## Proposed: BeamCalendar

**beamCalendarId** int(10) unsigned NOT NULL AUTO\_INCREMENT PRIMARY KEY,

**run** varchar(7) NOT NULL, — e.g. '2016-04', same as the run column in v\_run

**beamStatus** varchar(24) NOT NULL, – e.g. 'User Mode', 'UM Special Beam', 'Start up/Machine dev', 'Shutdown', ...

startDate datetime NOT NULL,

endDate datetime NOT NULL

Also: BLSession.beamCalendarId FK

Also: BeamCalendar apId(10) unsigned – see next slide



## Not yet proposed: AP

apId int(10) unsigned auto\_increment primary key

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- apNumber int(10) unsigned
- startTime datetime
- endTime datetime



## Proposed: BLSampleImageMeasurement

**blSampleImageMeasurementId** int(11) unsigned auto\_increment NOT NULL,

blSampleImageId int(11) unsigned NOT NULL,

blSubSampleId int(11) unsigned,

startPosX double,

startPosY double,

endPosX double,

endPosY double,

**blTimeStamp** datetime

