FlywheelTools:

Data Curation and Manipulation on the Flywheel Platform

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ABSTRACT

The recent and growing focus on reproducibility in neuroimaging studies has led many major
academic centers to use cloud-based imaging databases for storing, analyzing, and sharing complex
imaging data. Flywheel is one such database platform that offers easily accessible, large-scale data
management, along with a framework for reproducible analyses through containerized pipelines. The
Brain Imaging Data Structure (BIDS) is a data storage specification for neuroimaging data, but
curating neuroimaging data into BIDS can be a challenging and time-consuming task. In particular,
standard solutions for BIDS curation are not designed for use on cloud-based systems such as
Flywheel. To address these challenges, we developed "FlywheelTools", a software toolbox for
reproducible data curation and manipulation on Flywheel. FlywheelTools includes two elements: *fw-*
heudiconv, for heuristic-driven curation of data into BIDS, and *flaudit*, which audits and inventories
projects on Flywheel. Together, these tools accelerate reproducible neuroscience research on the
widely used Flywheel platform.

KEYWORDS: neuroimaging, neuroinformatics, BIDS, curation, Python

1   INTRODUCTION

Many fields in science are grappling with failures of scientific reproducibility (Botvinik-Nezer et al. 2020). Given the high dimensionality of the data, the need for complex image processing, and a plethora of analytic techniques, this crisis is particularly acute for neuroimaging research. Increasingly, the field has recognized that unstructured filesystems are a major source of non-reproducible practices. As such, major academic centers and large consortia have increasingly adopted platforms that leverage database technologies that have become standard in other fields. In addition to providing functionality for searching and categorizing complex source data, imaging databases enhance reproducible research by providing a clear audit trail of image processing applied to the data and its results, including both derived images and other data. Widely used imaging databases include Collaborative Informatics Neuroimaging Suite (COINS) (Landis et al. 2016), eXtensible Neuroimaging Archive Toolkit (XNAT) (Herrick et al. 2016), Longitudinal Online Research and Imaging System (LORIS) (Vaccarino et al. 2018), and others (Book et al. 2016; Helmer et al. 2011; Rogovin et al. 2020; Helmer et al. 2011; Poldrack and Gorgolewski 2017). More recently, the commercial platform Flywheel has seen growing adoption by major academic imaging centers (e.g., Stanford, Columbia, Duke, and Penn) due to its modern technology, ease of use, and scalability.

Most neuroimaging databases now leverage the standards defined by the Brain Imaging Data Structure (BIDS) (Gorgolewski et al. 2016). BIDS is an open-source standard for neuroimaging data organization that specifies how files should be named, how directories should be organized, and how metadata should be structured. As such, BIDS provides users with a well-documented format to understand both imaging data and metadata. Importantly, as BIDS provides a transparent format for recording imaging parameters and key aspects of the experimental design, BIDS enhances both data accessibility and data sharing.

Furthermore, BIDS allows users to leverage BIDS-apps — image processing pipelines, such as fMRIPrep, c-Pac, and QSIprep, that read the metadata defined by BIDS (Esteban et al. 2019; Craddock et al. 2013; Cieslak et al. 2020). As BIDS-apps can auto-configure to ensure that analytic parameters are appropriate for the input data provided, they dramatically reduce barriers to implementing best practices in image processing. Furthermore, containerized BIDS-apps encompass all software dependencies, further enhancing reproducibility.

On a filesystem, conversion of raw DICOM images to NIfTIs that conform to BIDS can be accomplished with a variety of tools including *HeuDiConv*, *dcm2bids*, and others. However, this crucial step, a process typically called "BIDS curation," is often difficult to implement within the database environment, as it requires a mechanism for converting data in hierarchical databases into BIDS. As BIDS curation is one of the very first steps performed on the data, lack of transparency in curation can impact the reproducibility of all subsequent steps. Here we introduce FlywheelTools, a software suite that provides flexible and reproducible methods for BIDS curation on the Flywheel platform. Documentation and code presented in this work can be found online at: https://fw-heudiconv.readthedocs.io/en/latest/.

2   METHODS

The FlywheelTools toolkit allows users to follow a reproducible workflow for BIDS curation and auditing of their data. This workflow typically includes: inspection of sequences collected during a study, design of a curation schema, implementation of that curation schema, and, finally, auditing and inspection of the curated data.

2.1   Programming Languages & Technologies

FlywheelTools is built primarily in Python 3.6 (Van Rossum and Drake 2009) to leverage Flywheel's
highly accessible Software Development Kit (SDK). Additionally, R 3.4.1 (R Core Team 2019) is
used for HTML report generation. For reproducibility and workflow management, the modules of
FlywheelTools are packaged in version-controlled software containers built and managed in Docker
(Merkel 2014). Lastly, the FlywheelTools package relies on users adopting BIDS to curate their data.
BIDS has rapidly evolved to become the directory standard in the neuroimaging community for
reproducible data organization. Importantly, BIDS is supported by a large community that
contributes to its development and adoption. Further, proposals for BIDS schema pass through a
rigorous testing process before being adopted. Software developers leverage this ubiquity by creating
BIDS-apps: analysis and processing pipelines that operate directly on BIDS datasets as inputs,
enhancing reproducibility and interoperability.

2.2   Flywheel

Flywheel is a data management and analysis platform that is tailored for neuroimaging research. The
platform focuses heavily on collaborative and reproducible science. User-facing components of the
platform itself are the web User Interface (UI), the Command Line Interface (CLI), the Flywheel
Software Development Kit (SDK), and the Application Programming Interface (API).

2.3   Flywheel Web UI

The web UI is accessible through any modern web browser. Through this point-and-click interface,
users are able to upload, view, download, and analyze data with ease. However, accomplishing tasks
with many repetitive steps or over a large number of participants/sessions can be tiresome and error-
prone. Alongside knowledge of navigating the web UI, many users also make use of the API and
SDK to manipulate and analyze data programmatically.

2.4   Flywheel API & SDK

Flywheel's database uses MongoDB for data storage and access, meaning that all Flywheel data are
represented by hierarchical relationships between document objects. This allows users to create and
store complex structures with ease, and query data rapidly (Banker 2011). To access these data,
Flywheel uses a RESTful Application Programming Interface (REpresentational State Transfer)
(Biehl 2016), making each document or data object accessible through a specific URL that a web
browser or SDK can access by requesting the data and waiting for a response from the server. The
Flywheel Python SDK[1] provides a powerful interface for inspecting and manipulating data through
this API. By standardising this underlying data model into Pythonic objects, the Flywheel SDK is
effectively an object relationship mapper, similar to the popular SQLAlchemy software.

2.5   Flywheel Data Model

Objects in Flywheel's data model follow a specific hierarchical structure — at the top level is a
Flywheel instance, a process that serves the API to an organization (for example, a neuroimaging
center). Within the Flywheel instance, there are multiple groups, which are typically labs or research
units that collaborate on one or more projects. Each project object can have one or many subjects (i.e.

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[1] Flywheel also provides a MATLAB SDK, however we use the term SDK in this work to refer to the Python SDK, which we use exclusively in FlywheelTools.

participants), and each subject can have one or many sessions (i.e. scanning visits). Within a session,
there may be one or many acquisition objects which represent the scanning sequences collected
during a particular scan or examination (e.g., sMRI, rs-fMRI, dMRI). Finally, the data files
associated with the sequence (e.g., NIfTIs or DICOMs) are attached to each acquisition. Note that a
file can additionally be attached to any object type, and each object can have metadata associated
with it. Hence, a "subject" object may have metadata associated with that participant (such as
demographic information) and may also have a text file attached to it (such as clinical data). A
notable exception to this hierarchical structure is the analysis object, which behaves in much the
same way as others but can be a child object of any other object, allowing researchers to create
analyses of entire projects, for example, each with their own associated metadata and files.
118
119 Abstracting this data model in Python results in simple hierarchical objects, each with methods for
120 handling metadata and files, and methods for accomplishing object-specific tasks like traversing the
121 hierarchical structure or running analyses. The modules of FlywheelTools make use of this data
122 model to accomplish a wide range of tasks.

2.6 Flywheel Gears

Flywheel encourages the use of pre-packaged computational workflows, called "gears". Gears are
run by virtual machines/containers using Docker and hence are version-controlled and
software/platform agnostic. Gears can accomplish tasks such as data manipulation, pre-processing,
and analysis. In addition to the existing gears available on the platform, users are able to package
their own software in a gear and use it for running analysis workflows on their Flywheel data via the
web UI or SDK. The complexity and frequency of the task guides if a task should be accomplished
using the web UI, programmatically using the SDK, or by wrapping it as a workflow into a gear.
Gears ingest existing Flywheel data (such as images or file attachments) as inputs to the workflow
and can be created with clickable configuration options. Once a workflow has completed running,
Flywheel collects any files remaining in the pre-defined output directory of the container and attaches
them to a resulting analysis object. The output of a gear (such as an HTML report or tabulated data)
can be viewed on the Flywheel UI, downloaded to disk for further sharing or analysis, or used as
input to a subsequent gear.
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3 RESULTS

FlywheelTools is implemented using the Flywheel SDK to enable easy inspection, curation,
validation, and audit of Flywheel data through a handful of user-friendly gears and command-line
interfaces. The first module of the package is called *fw-heudiconv* and is largely inspired by the
popular Heuristic DICOM Converter package (Halchenko et al. 2018). *fw-heudiconv* is a multi-part
toolbox for reproducible curation of neuroimaging data into BIDS on Flywheel. The second module,
flaudit, is a tool for auditing a Flywheel project, giving users an overview of the key elements of their
data set.

3.1 FW-HEUDICONV

147 The first tool, *fw-heudiconv*, is a multi-purpose command-line interface and Flywheel gear designed
148 for BIDS curation on Flywheel (**Figure 1**). It is designed to be intuitive, flexible, and reproducible.

3.1.1 Architecture & Design

fw-heudiconv is inspired in large part by the Heuristic DICOM Converter (*HeuDiConv*) package, and
shares much of its design practices. To curate data into BIDS format, *fw-heudiconv* first considers
DICOM data to be the "ground truth" and builds its curation approach using data in the DICOM
headers. On Flywheel, when DICOMs are added to the database, either through manual upload or
automatically from a linked scanner. The DICOMs are then automatically converted into NIfTI files
by Flywheel's automated gears. The result is an acquisition object with both DICOMs and one or
more NIfTIs. Ultimately, *fw-heudiconv* only has permission to manipulate metadata associated with a
NIfTI file. By not manipulating DICOMs or their associated metadata, BIDS curation can safely be
reproduced from ground truth data.

fw-heudiconv can be downloaded as a Python command-line interface from the Python Package
Index using *pip*. It is also available as a point-and-click gear that is managed by Docker
containerization. This containerization allows for reproducible version control, as every computation
can be recorded, including information about the software, OS, and algorithm versions. There are a
number of commands available in *fw-heudiconv*, and each of them starts by querying data from
Flywheel. Users can filter their queries to operate on an entire Flywheel project, a subset of subjects,
or a subset of sessions. Notably, with the `--dry-run` option, each command has the ability to test
and evaluate its effects without actually manipulating metadata in the Flywheel database or writing
data to disk. Below, we consider each of the five available commands.

3.1.1.1 fw-heudiconv-tabulate

The tabulate tool is used to parse and extract DICOM header information in a project (or within a
filtered subset of that project) and compile these data into a table for the user to examine. By
collecting DICOM header information into a tabular format, the tabulate tool gives users a
comprehensive overview of the different scanning sequences that have been collected in the query,
including the sequence parameters. Additionally, users have the option to limit the tabulation to a
unique combination of common DICOM header fields, which significantly decreases the complexity
of the table. When used at the command line, the table produced by this command is written to a
local disk. As a gear on Flywheel, the table is automatically saved in the output section of the gear.

3.1.1.2 fw-heudiconv-curate

The curate tool is used to curate a dataset on Flywheel into BIDS format. Much like *HeuDiConv*,
curation is accomplished through the use of a heuristic: a Python file that programmatically defines
the templates for a range of BIDS-valid filenames, and defines the boolean logic that would assign a
given scanning sequence to each template. This boolean logic is usually based on the sequence
information users find in the tabulation of sequences, but all fields available in the DICOM header
can be used to determine which template a particular file can be assigned to. Additionally, the curate
tool can be used to manipulate BIDS metadata that may need to be added to the dataset. The process
of curation only manipulates the BIDS metadata of NIfTI files, and hence can be repeated or updated
at any time at the user's discretion.

3.1.1.3 fw-heudiconv-export

188   The export tool is used to export a BIDS dataset on Flywheel to disk. It can also be used by other
189   gears and scripts to quickly and easily extract their BIDS data into the workspace of their analysis
190   pipeline.

3.1.1.4 fw-heudiconv-validate

The validate tool is a wrapper around the popular BIDS Validator package and is used to check if the
applied curation results in a BIDS-valid dataset. After exporting a dataset with *fw-heudiconv-export*,
the validate tool runs the BIDS Validator on the dataset and returns the verbose output of the errors
and warnings given by the BIDS Validator. Additionally, the results of the validator can be tabulated
for easy inspection. On the Flywheel GUI, *fw-heudiconv-validate* also displays a green check mark in
the analysis tab for a successful validation, and a red check mark otherwise, allowing for quick visual
inspection of BIDS curation status for each session.

199   3.1.1.5 fw-heudiconv-clear

200   The clear tool is used to clear BIDS information cleanly and safely from the project or subjects and
201   sessions queried. This can be useful when a user wants to rerun the curation. The previously created
202   persistent fields can be removed by running *fw-heudiconv-clear* before re-curating.

203   3.1.2 The Heuristic File

The heuristic file is a Python file used as input to the *fw-heudiconv-curate* command. The file
instructs *fw-heudiconv* on how to programmatically sort and parse through each acquisition object in
Flywheel and assign it to a valid BIDS naming template. This is done by checking the attributes of a
list of *seqInfo* objects — which are generated from each DICOM's header information — against
user-defined boolean rules. For example, if a T1-weighted image is present in a dataset, the user may
define a string with a BIDS-valid naming template for this type of file, such as:

```
210    t1w = 'sub-{SubjectLabel}_ses-{SessionLabel}_T1w.nii.gz'
```

Where the SubjectLabel and SessionLabel portions are expected to be automatically generated for
each subject and session in the dataset. After the DICOM SeriesDescription field is added to the
SeriesDescription attribute of *seqInfo*, the user can create a simple boolean expression to check if the
string 'T1w' is in the SeriesDescription. If such a rule is met, this acquisition and its NIfTI file will
be assigned to the T1-weighted image naming template. The NIfTI file will ultimately have this
BIDS naming added to its metadata and be named correctly when exported to a filesystem. In more
complex naming scenarios, *fw-heudiconv* can flexibly use boolean expressions involving any number
of *seqInfo* attributes, which the user can access in the output of *fw-heudiconv-tabulate*.

In addition to setting naming templates, the heuristic file can also be used to hard-code and assign
metadata in BIDS. These data are hard-coded into the metadata of the file object on Flywheel and are
assigned by using specially reserved functions and keywords in *fw-heudiconv*. For example, the
heuristic file can be used to point fieldmap scans to their intended sequences using a list:

```
223    IntendedFor = {
```

```
224    fieldmap1: ['sub-{SubjectLabel}_ses-{SessionLabel}_task-rest_bold.nii.gz']
```

```
225    }
```

By reserving select keywords for functions and metadata, heuristic files become versatile tools for
defining and manipulating a wide array of metadata in Flywheel BIDS curation.

Importantly, because this heuristic file is plain text Python code, users are able to version control
their files using Git and share these files via Github. Finally, when run on Flywheel as a gear, the

heuristic file is automatically attached as an input to the analysis object created by *fw-heudiconv-*
curate, allowing users to easily access the version history of their curation.

3.1.3 Curation Workflow

For most users, the curation workflow follows the sequence detailed above (**Figure 2**). After
DICOMs have been converted to NIfTIs, users can then begin by running *fw-heudiconv-tabulate* to
gather the information stored in the DICOM headers necessary for creating a heuristic. Once the
tabulation has been completed, the output file can be opened by any program that can read tabular
data. At this stage, users can begin creating a heuristic file and running *fw-heudiconv-curate*, using
the `--dry-run` flag to test the heuristic changes incrementally with informative logging. When
satisfied, users can simply remove the `--dry-run` flag to apply the changes. The user can then use
fw-heudiconv-validate to run the BIDS validator on the dataset or start over by removing all BIDS
metadata with *fw-heudiconv-clear*.

If *fw-heudiconv* is run from the Flywheel GUI, each of the commands is available as a Flywheel gear.
This option is beneficial for data provenance, as all of a gear's commands and inputs, as well as
outputs and logs, are stored and attached to each gear run.

3.2 FLAUDIT

The second module of FlywheelTools is a Flywheel project auditor, named *flaudit*. The module is
intended to give Flywheel users a broad understanding of their entire Flywheel project, by
summarizing the available data and illustrating analysis workflows. The output of this module, a
portable HTML report, presents this information using a number of visualizations built in R
Markdown using HTML, Javascript, and ggplot2, in two main sections: project overview and project
completeness.

3.3 Architecture & Design

253 Using internal machinery similar to *fw-heudiconv-tabulate*, *flaudit* loops over existing data in a
254 project and tabulates information about scanning sequences, BIDS metadata, and gear analyses that
255 have been run. These three tables are saved internally and then passed as input to an R markdown
256 script that generates an interactive HTML report. The data are also saved as output for the user to
257 further access and analyze in their software of choice.

3.4 Flaudit: Project Overview

The overview section of the *flaudit* report provides a numerical overview of sequences, BIDS data,
gear runs, and gear runtimes.

The first visualization uses the sequence data input to create a bar chart visualizing the names of the
different sequences acquired across the entire Flywheel dataset. This visual is accompanied by an
interactive table that users can search to compare values (**Figure 3**).

Next, using the BIDS metadata input, the report provides an interactive tree viewer to examine BIDS
curation. In the tree, the nodes branch out from the project to show each sequence acquisition. For
each acquisition, if the data has been curated into BIDS, the node itself can also branch out to show a
BIDS name template, demonstrating what BIDS name that sequence has been given. Hovering over
the BIDS name will display the number of subjects whose data have been named as such (**Figure 4**).

Finally, using the gear analysis data as input, the last section of the overview enumerates the gear
analyses that have been run successfully on any session within the project, and enumerates the
runtimes for these processes. The results are visualized in a bar chart (**Figure 5**).

3.5   Flaudit: Project Completeness

As an optional input, *flaudit* allows users to specify a *template* subject — a subject from the Flywheel
project who serves as an exemplar for other subjects to be compared against. This subject should be
chosen based on the fact that they have both complete input data and analyses. This allows *flaudit* to
determine if other subjects in the project have equally complete data or are missing specific raw data
or analytic output. The project completion section of the *flaudit* report consists of three interactive
tables.

In the first table, it's assumed that the template subject has acquired a complete set of imaging
sequences. These sequences are listed as columns in the table. Each subsequent row is a subject in the
project, and each value in the table is a boolean (complete or incomplete) indicating if that subject
has each sequence. The table is searchable, meaning that users can simply filter each column for
"incomplete" to learn which subjects do not have the same data as the template (**Figure 6A**).
Likewise, the second table illustrates the completeness of BIDS data for other subjects in comparison
to the template (**Figure 6B**). In this case, rows indicate subjects while columns delineate the
specified BIDS naming template. Lastly, the third table illustrates completeness of analytic gear runs.
Researchers can use this table to compare the analytic output of all other subjects in the project to the
analysis pipelines run for the template subject. To ensure uniform versions of pipeline software, the
version of a pipeline that was used for each subject must match that of the template subject (**Figure
6C**).

4   DISCUSSION

FlywheelTools provides new capabilities for the popular and powerful Flywheel platform, allowing
researchers to maximize reproducibility and enhance scalability. Specifically, *fw-heudiconv* provides
users a flexible and reproducible way of curating data into BIDS on Flywheel. Complementary
function is provided by *flaudit*, which provides intuitive visual reports of raw, curated, and processed
data.

Flywheel has been rapidly adopted by major imaging centers due to its ease of use, extensive
functionality, scalability, and emphasis on reproducible research. Despite these strengths, at present
there have been limited options for conversion of imaging data to BIDS format on Flywheel. This
step is absolutely critical, as BIDS provides a standardized format for important imaging metadata.
Notably, initial curation to BIDS has frequently been an important gap in workflows for reproducible
research.

Accordingly, *fw-heudiconv* provides critical functionality for reproducible and flexible BIDS curation
on Flywheel. The combination of containerized code and heuristics that are version controlled with
git maximizes reproducibility, ensuring that all curation steps have a clear audit trail. Furthermore,
the flexible architecture employed by *fw-heudiconv* allows workflows to be updated to accommodate
both new scanning protocols and the evolving specifications of the BIDS standard.

Once data are curated with *fw-heudiconv*, *flaudit* allows users to audit the data in a Flywheel project.
Specifically, *flaudit* provides intuitive summaries at each stage of a typical workflow, concisely
visualizing raw data, curated data in BIDS, and data processed by containerized analytic gears. These

accessible reports allow users to rapidly assess the overall organizational state of a project, while
interactive tables allow for more granular inspection of data. This approach facilitates understanding
the diverse data types typically collected in multi-modal imaging studies.

There are of course limitations of FlywheelTools. First, it should be acknowledged that
FlywheelTools is built for the Flywheel platform, and as such does not generalize to other imaging
databases that are in use. However, given the rapid adoption of this platform by the imaging
community, we anticipate that this toolkit will fill an important need for the many large research
institutions that rely upon Flywheel. Second, some understanding of Python is necessary to build the
heuristic for *fw-heudiconv*. We attempt to minimize this issue by providing both extensive
documentation and heuristic templates for various uses of *fw-heudiconv*[2], but usage is ultimately a
programming task.

FlywheelTools provides essential functionality to the Flywheel platform. The flexible toolkit allows
for curation and description of complex imaging studies. Taken together, the toolkit is designed to
accelerate reproducible imaging research at scale.

5   CONFLICT OF INTEREST

327 The authors declare that the research was conducted in the absence of any commercial or financial
328 relationships that could be construed as a potential conflict of interest.

6   AUTHOR CONTRIBUTIONS

330 T.M.T. and M.C. contributed to the design and implementation of the code and software. T.D.S.,
331 M.B., and M.C. supervised writing of the manuscript. A.A., M.C., E.R.B., D.D. and W.T. provided
332 substantial software use-cases, software feature requests, test data, and critical bug reports. K.M. and
333 S.L. assisted with software documentation. M.A.E., G.K.A., P.AC., J.A.D., and T.D.S. were involved
334 in proposing, planning, and supervising all the work.

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[2]https://fw-heudiconv.readthedocs.io/en/latest/index.html

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10   FIGURES

Figure 1: BIDS-app workflow. BIDS curation on file systems is a common task that can be accomplished by existing tools (heudiconv, dcm2bids, etc) or manually, but mechanisms for BIDS curation on many cloud databases have yet to be developed. FlywheelTools provides this functionality for the Flywheel platform.

Figure 2: FlywheelTools workflow. Users first use the tabulate tool to extract sequence information from their data, which they use to develop a heuristic that delineates how sequences are mapped into BIDS. After this, they use the curate tool to convert their data into BIDS, and the validate tool to assess their curation. The export tool can be used to export their BIDS data as necessary.

Figure 3: Enumeration of available sequences in a flywheel project. Panel (**A**) plots the count of
files in each collected sequence; in this example, there are 60 files collected for the B0map sequence,
as there are 20 subjects and 3 B0map sequences. Panel (**B**) shows the accompanying interactive table.

403
404 **Figure 4: Interactive tree diagram illustrating BIDS curation.** The tree shows how each sequence
405 has been curated into BIDS format; users can hover their mouse over each leaf to show how many
406 files have been curated into each BIDS filename template.

Figure 5: Enumeration of gear runs in a Flywheel project. The number of gear runs is shown for
various gears. For each gear, the percent of completed versus failed runs is shown. For example, 95
percent of the subjects (n=19) were successfully run through fMRI-prep.

Figure 6: Project completeness tables compared to the template participant in a Flywheel project. Panel (**A**) compares the sequences available for each participant to the template subject and identifies missing sequences. For example, this table illustrates that subjects cec4ba54 and f53cd86f did not have DWI sequences collected. Panel (**B**) similarly shows completeness of BIDS curation. As expected, the two participants who did not have DWI sequences (in **A**) did not have diffusion data curated into BIDS. Panel (**C**) shows gear run completion; here, flaudit reports that the same two participants that lacked DWI data did not have a successful run of QSIPrep. Finally, the report notes that participant f53cd86f did not yet complete fMRIPrep or XCPEngine successfully.