TemplateFlow: FAIR-sharing of multi-scale, multi-species brain models

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Abstract Reference anatomies of the brain and corresponding atlases play a central role in experimental neuroimaging workflows and are the foundation for reporting standardized results. The choice of such references —i.e., templates— and atlases is one relevant source of methodological variability across studies, which has recently been brought to attention as an important challenge to reproducibility in neuroscience. *TemplateFlow* is a publicly available framework for human and nonhuman brain models. The framework combines an open database with software for access, management, and vetting, allowing scientists to distribute their resources under FAIR —findable, accessible, interoperable, reusable— principles. *TemplateFlow* supports a multifaceted insight into brains across species, and enables multiverse analyses testing whether results generalize across standard references, scales, and in the long term, species, thereby contributing to increasing the reliability of neuroimaging results.

Brains are morphologically variable, exhibiting diversity in such features as overall size (***Lüders et al., 2002***), sulcal curvature (***Tosun et al., 2015***), and functional topology (***Tavor et al., 2016***; ***Mars et al., 2018***). Morphological variability manifests not only in differences between brains but also in the way that a brain changes across its lifespan, as it is remodelled by development, aging, and degenerative processes (***Courchesne et al., 2000***; ***Good et al., 2001***; ***Sowell et al., 2003***). These morphological differences often correspond with the effects of interest in neuroimaging studies and hinder direct spatial comparisons between brain maps (***Brett et al., 2002***). The substantial variability within and between individual brains necessitates a means of formalizing population-level knowledge about brain anatomy and function. Neuroscientists have answered this need by creating brain atlases as references for understanding and contextualizing morphological variability. Atlases map landmarks, features, and other knowledge about the brain as annotations that are consistent across individual brains.

The development of atlases in neuroscience has accelerated knowledge discovery and dissem-

ination. Early endeavors, epitomized by the groundbreaking work of ***Brodmann*** (***2006***, originally published in German in 1909) and complemented by ***Von Economo and Koskinas*** (***2008***, originally published in German in 1925), leveraged careful scrutiny of microanatomy and cytoarchitectonic properties in small numbers of brains. Talairach's assiduous postmortem examination of a single brain (***Talairach et al., 1957***) remarkably incorporated stereotaxy by defining three spatial reference axes over the brain that allowed anchoring neural landmarks to coordinates. This first stereotaxic atlas saw wide use with a later, improved version (***Talairach and Tournoux, 1988***). Stereotaxy also prompted the development of the earliest surgical neuronavigation systems. ***Schurr and Merrington*** (***1978***) developed a stereotaxic apparatus to surgically induce targeted brain lesions on cats. This work informed early sectional atlases of the rodent (***Paxinos and Watson, 1997***) and macaque (***Martin and Bowden, 2000***) brains.

On account of its implicit stereotaxy, its capacity to image the entire brain, and its non-invasive acquisition protocols, magnetic resonance imaging (MRI) has revolutionized neuroscience in general and the atlasing endeavor (***Evans et al., 2012***) in particular. In combination with software instruments' progress to map homologous features between subjects supported by regular grids (***Avants et al., 2008***) or reconstructed anatomical surfaces (***Robinson et al., 2014***), MRI has enabled researchers to create population-average maps of a particular image modality and/or particular sample with relative ease. These maps, called "templates", are typically created by averaging features across individuals that are representative of the population of interest to a study (***Dickie et al., 2017***). As a result, atlasing endeavours have been made contingent on templates, and have shifted away from the search for a single universal neuroanatomical pattern, instead making use of increasingly large samples with the aim of representing a population average of the distribution of morphological patterns (***Evans et al., 1993***). Although neurotypical human adults have historically been the most comprehensively templated brains (***Evans et al., 1993***; ***Mazziotta et al., 1995***, ***2001***; ***Evans et al., 2012***; ***Landman et al., 2012***; ***Satterthwaite et al., 2016***), researchers have also generated templates and atlases for diseased (***Dickie et al., 2015***), infant (***Matsuzawa et al., 2001***; ***Fonov et al., 2011***; ***Shi et al., 2011***), and elderly (***Buckner et al., 2004***) human populations. Similarly, nonhuman MRI templates have seen parallel development, e.g., rodents (***Calabrese et al., 2013***; ***Szulc et al., 2015***), and primates (***Schilling et al., 2017***; ***Jung et al., 2021***). Advancing beyond the volumetric constraints of stereotaxy, researchers of the primate neocortex have also devised standard spaces based on geometric reconstructions of the cortical surface (***Fischl et al., 1999***). This surface-based approach has the advantage of respecting the intrinsic topology of cortical folds, a development that has led to further improvements in spatial localization (***Van Essen et al., 2012***; ***Coalson et al., 2018***).

Such resources as atlases and templates, which provide standardized prior knowledge, have become an indispensable component of modern neuroimaging data workflows for two cardinal reasons. First, group inference in neuroimaging studies requires that individuals' features are aligned into a common spatial frame of reference where their location can be called standard (***Brett et al., 2002***). Second, templates engender a stereotaxic coordinate system in which atlases can be delineated or projected. Associating atlases with template coordinates also facilitates the mapping of prior population-level knowledge about the brain into images of individual subjects' brains (for instance, to sample and average the functional MRI signal indexed by the regions defined in an atlas; ***Yeo et al.*** (***2011***)). Because they are integral to analytic workflows, the most widely-used templates and atlases are typically distributed along with neuroimaging software libraries. Alternatively, researchers distribute their templates through, e.g., the *NeuroImaging Tools and Resources Collaboratory* [NITRC; RRID:SCR_003430], institutional websites, or data storage systems such as FigShare [RRID:SCR_004328] or Dryad [RRID:SCR_005910]). However, using the default templates of their analyses' software toolbox is the most common practice, as shown by ***Carp*** (***2012b***) in a review of 241 functional MRI studies.

In sum, a number of challenges have derived from management, stewardship, distribution, reuse and reporting of templates that merit attention. In an early perspective, ***Van Essen*** (***2002***)

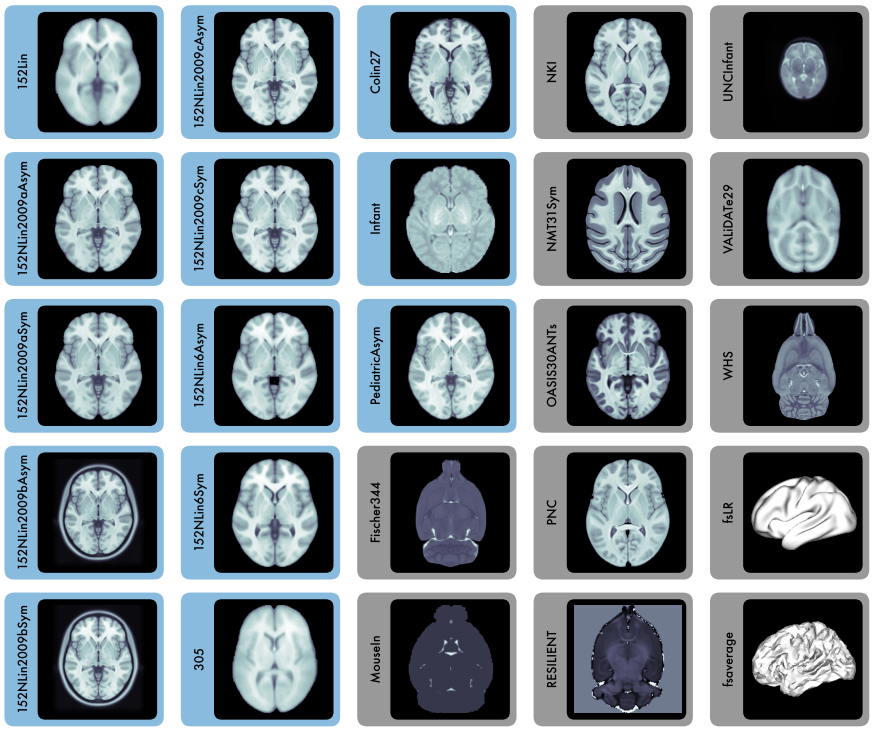

Figure 1. Representative views of 25 templates currently available in the *TemplateFlow Archive*. The 13 templates highlighted in blue are constituents of the Montreal Neurological Institute (MNI) portfolio. `WHS` (Waxholm space), `Fischer344`, `RESILIENT`, and `MouseIn` correspond to rodent templates. `fsaverage` and `fsLR` are surface templates; the remaining templates are volumetric. Each template is distributed with atlas labels, segmentations, and metadata files. The 25 templates displayed here are only a small fraction of those created as stereotaxic references for the neuroimaging community.

called for connecting templates in an aggregation of databases with "powerful and flexible options for searching, selecting, and visualizing data" and stressed the importance of resource accessibility. *TemplateFlow* provides a framework that satisfies all of the aforementioned desiderata while following the "Findability, Accessibility, Interoperability, and Reusability (FAIR) Guiding Principles" (Box 1; ***Wilkinson et al., 2016***). Following the FAIR Principles, *TemplateFlow* effectively decouples standardized spatial data from software libraries while affording processing and analysis workflows (e.g. ***Esteban et al., 2017***, ***2019***) with the necessary flexibility to select the most appropriate template available. *TemplateFlow* comprises a cloud-based repository of human and nonhuman imaging templates —the "*TemplateFlow Archive*", Figure 1— paired with a Python-based library —the "*TemplateFlow Client*"— for programmatically accessing template resources. The resource is complemented with a "*TemplateFlow Manager*" tool to upload new or update existing resources. When adding a new template, the *Manager* initiates a peer-reviewed contribution pipeline where experts are invited to curate and vet new proposals. These software components, as well as all template resources, are version-controlled. Therefore, not only does *TemplateFlow* enable "off-the-shelf" access to templates by humans and machines, it also permits researchers to share their resources with the community. To implement several of the FAIR Principles, the *TemplateFlow Archive* features a tree-directory structure, metadata files, and data files following an organization inspired by the Brain Imaging Data Structure (BIDS; ***Gorgolewski et al., 2016***). The online documentation hub and the resource browser located at TemplateFlow.org provide further details for users.

Results

BIDS-inspired structure for template and atlas archival following FAIR Principles

BIDS prescribes a file naming scheme comprising a series of key-value pairs (called "entities"). Mirroring BIDS' patterns for participants, each template is associated with an identifier, which is an alphanumeric label. Template identifiers are unique across the *Archive*, and signified with the key `tpl-` (e.g., `tpl-MNI152Lin`), which is analogous to `sub-` of BIDS. Hence, every template and all

Box 1. The FAIR Guiding Principles

To be **Findable**:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be **Accessible**:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
  - A1.1. the protocol is open, free, and universally implementable
  - A1.2. the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be **Interoperable**:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

To be **Reusable**:

- R1. (meta)data are richly described with a plurality of accurate and relevant attributes
  - R1.1. (meta)data are released with a clear and accessible data usage license
  - R1.2. (meta)data are associated with detailed provenance
  - R1.3. (meta)data meet domain-relevant community standards

(Reproduced from ***Wilkinson et al., 2016***, Box 2)

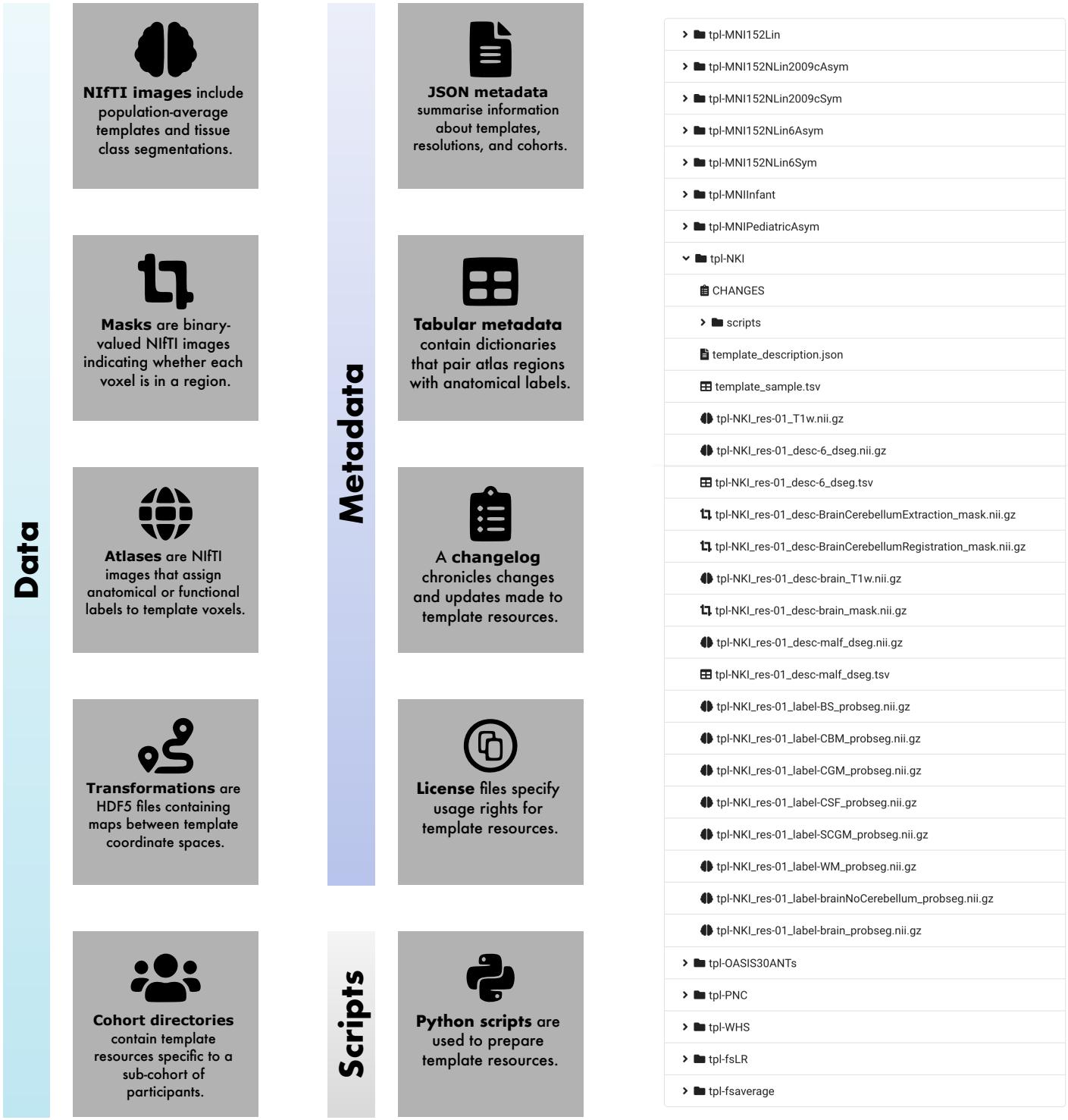

Figure 2. The *TemplateFlow Archive* contains template resources. Left, common file formats included in the *TemplateFlow Archive*. Right, view of the *TemplateFlow Archive*'s browser, accessible at TemplateFlow.org, with a single template resource directory expanded. Template data are archived using a BIDS-like directory structure, with top-level directories for each template. Each directory contains image files, annotations, and metadata for that template. Following BIDS specifications, volumetric data are stored in NIfTI-1 format. Further surface-based data types are supported with GIFTI (surfaces) and CIFTI-1 (mixed volumetric-and-surface data).

associated metadata, atlases, etc. are assigned a unique and persistent identifier (Box 1, F1). The adaptation of BIDS to the domain of templates and atlases affords the tool with a robust implementation of the principles I1-3 in Box 1. For each template, the *TemplateFlow* database includes reference volumetric template images (e.g., one T1-weighted MRI), a set of atlas labels and voxel-wise annotations defined with reference to the template image, and additional files containing the template and atlas metadata. Correspondingly, *TemplateFlow* allows surface-based resources such as average features, geometry files, annotations, or metadata. The only requirement for feature averages and atlases sharing a unique template identifier is that they must be spatially in register, regardless of the data sampling strategy (i.e., volume, surface, or mixed, and corresponding resolution or mesh density). Although the most widely used templates generally represent MRI-derived features, *TemplateFlow* is not limited to any specific set of modalities. Supplementary Table S1 has been programmatically generated by the accompanying code examples, and enumerates the templates currently distributed with the *Archive* indicating their corresponding unique identifiers and including a short description.

Template resources are described with rich metadata (Box 1, F2 and R1), ensuring that the data usage license is clear and accessible (Box 1, R1.1), data and metadata are associated with detailed provenance (Box 1, R1.2), and data and metadata follow a domain-relevant structure transferred from the neuroimaging community standards of BIDS (R1.3). Figure 2 summarizes the data types and metadata that can be stored in the *Archive*. Figure 3 provides an overview of the *Archive*'s metadata specification, showing that metadata clearly and explicitly include the identifier of the data they describe (Box 1, F3). Data and metadata are retrievable using several open, free, standard communications protocols without need for authentication (Box 1, A1) by using *DataLad* (***Halchenko et al., 2021***). Cloud storage for the *Archive* is supported by the Open Science Framework (osf.io) and Amazon's Simple Storage Service (S3). Version control, replication, and synchronisation of template resources across filesystems is managed with *DataLad*. Leveraging *DataLad*, metadata are stored on GitHub, ensuring accessibility to metadata even when corresponding data are no longer available (Box 1, A2). *DataLad* is based on *Git* and *Git-Annex*, which index all data and metadata (Box 1, F4).

TemplateFlow **provides humans and machines with flexible and granular access to templates**

TemplateFlow's Python client provides human users and software tools with reliable and programmatic access to the archive. The client can be integrated seamlessly into image processing workflows to handle requests for template resources on the fly. It features an intuitive application programming interface (API) that can query the *TemplateFlow Archive* for specific files (Figure 4). The BIDS-inspired organization enables easy integration of tools and infrastructure designed for BIDS (e.g., the Python client uses *PyBIDS*; ***Yarkoni et al., 2019***). To query *TemplateFlow*, a user can submit a list of arguments corresponding to the BIDS-like key-value pairs in each entity's file name (see Online Methods).

To integrate template resources into neuroimaging workflows, traditional approaches required deploying an oftentimes voluminous tree of prepackaged data to the filesystem. By contrast, the *TemplateFlow* client implements lazy loading, which permits the base installation to be extremely lightweight. Instead of distributing neuroimaging data with the installation, *TemplateFlow* allows the user to dynamically pull from the cloud-based storage only those resources they need, as they need them. After a resource has been requested once, it remains cached in the filesystem for future utilization.

We demonstrate benefits of centralizing templates in general, and the validity of the *TemplateFlow* framework in particular, via its integration into *fMRIPrep* (***Esteban et al., 2019***), a functional MRI preprocessing tool. This integration provides *fMRIPrep* users with flexibility to spatially normalize their data to any template available in the *Archive* (see Box 2). This integration has also enabled the development of *fMRIPrep* adaptations, for instance to pediatric populations or rodent

```
{
  "Authors": [
    "Fonov V",
    "Evans AC",
    "Botteron K",
    "Almli CR",
    "McKinstry RC",
    "Collins DL"
  ],
  "Curators": [
    "Esteban O"
  ],
  "Identifier": "MNIPediatricAsym",
  "License": "MIT-derived. See LICENSE file",
  "Name": "MNI's unbiased standard MRI template for
           pediatric data from the 4.5 to 18.5y age
           range",
  "RRID": "SCR_008796",
  "ReferencesAndLinks": [
    "https://doi.org/10.1016/j.neuroimage.2010.07.033",
    "https://doi.org/10.1016/S1053-8119(09)70884-5",
    "http://nist.mni.mcgill.ca/?p=974",
    "https://doi.org/10.1007/3-540-48714-X_16"
  ],
  "TemplateFlowVersion": "1.0.0",
  "cohort": {
    "1": {
      "age": [
        4.5,
        18.5
      ],
      "name": "whole age range",
      "units": "yr"
    },
    "2": {
      "age": [
        4.5,
        8.5
      ],
      "name": "prepuberty",
      "units": "yr"
    },
  . . .
  },
  "res": {
    "1": {
      "origin": [
        -98.0,
        -134.0,
        -72.0
      ],
      "shape": [
        197,
        233,
        189
      ],
      "zooms": [
        1.0,
        1.0,
        1.0
      ]
    },
  . . .
  }
}
```


General metadata

Field	Type	Description
`Authors`	Array (String)	Names of authors who created the template.
`Curators`	Array	Names of TemplateFlow curators who contributed or manage the dataset.
`Identifier`	String	Unique human-readable template identifier within TemplateFlow.
`License`	String	License under which template resources are available.
`Name`	String	Full descriptive name of the template.
`RRID`	String	Research Resource Identifier for the TemplateFlow dataset.
`ReferencesAndLinks`	Array	Publications to reference when using the template, and salient links for template information.
`TemplateFlowVersion`	String	Version of TemplateFlow under which the dataset was distributed.

Cohort metadata

Field	Type	Description
`cohort`	Object	Top-level field containing all cohort metadata objects.
`1, 2, ...`	Object	Cohort identifiers. Each has a subdirectory in the template data directory, and each has a metadata object nested in the `cohort` field.
`age`	Array (Number)	2-tuple array indicating the lower and upper bounds for participant age in the cohort, if the cohorts are stratified by age.
`name`	String	Full descriptive name of the cohort..
`units`	String	Units for cohort age bounds.

Resolution metadata

Field	Type	Description
`res`	Object	Top-level field containing all resolution metadata objects.
`1, 2, ...`	Object	Resolution identifiers. Each has a metadata object nested in the `res` field. The metadata for each resolution apply to all images whose name includes `res-<identifier>`. The identifier itself does not necessarily correspond to the voxel size.
`origin`	Array	(x, y, z) spatial location of the voxel origin relative to the physical origin in mm.
`shape`	Array	(x, y, z) shape of the image in voxels.
`zooms`	Array	(x, y, z) size of each voxel in mm.

Figure 3. Overview of the metadata specification of the *TemplateFlow Archive*. *TemplateFlow*'s metadata are formatted as JavaScript Object Notation (JSON) files located within each template set. An example `template_description.json` metadata file is displayed at the left for `MNIPediatricAsym`. In addition to general template metadata, datasets can contain cohort-level and resolution-level metadata, which are nested within the main metadata dictionary and apply only to subsets of images in the dataset.

imaging (***MacNicol et al., 2021***), using suitable templates from the archive. The uniform interface provided by the BIDS-like directory organisation and metadata enables straightforward integration of new templates into workflows equipped to use *TemplateFlow* templates. Further examples of tools leveraging *TemplateFlow* include *MRIQC* (***Esteban et al., 2017***) for quality control of MRI; *PyNets* (***Pisner and Hammonds, 2020***), a package for ensemble learning of functional and structural connectomes; *ASLPrep* (***Adebimpe et al., 2021***), an ASL pre-processing pipeline that makes use of *TemplateFlow* through *sMRIPrep* —the spin-off structural pipeline from *fMRIPrep*;— and *NetPlotBrain* (***Thompson and Fanton, 2021***), which uses *TemplateFlow* to display spatially standardized brain network data.

TemplateFlow eases the dissemination of templates and opens their vetting and maintenance to the community

Beyond redistributing the templates most commonly used in the literature, the resource has the vision of becoming a centralized and standard way for researchers to disseminate their new templates. *Templateflow*'s pipeline for submission of new templates integrates peer-review with minimal technical overhead. This review process is proposed as a complement to the traditional assessment of template resources prior to publication, in which reviewers and editors focus on academic merit over accessibility and reusability potential. This submission pipeline is easily initiated with the Python-based *TemplateFlow Manager*, further described in the Online Methods.

TemplateFlow's management infrastructure also eases maintenance. The lack of infrastructure for templates and atlases has given rise to static development modes where templates are packaged once and rarely revised. As a result, templates and atlases have remained outside version control because it is considered too onerous and requires informatics expertise that may exceed the resources of research teams. Although uncommon, errors in template and atlas resources have nonetheless been reported (e.g., ***Rohlfing, 2013***; ***Halchenko, 2013***), and the common denominator across these instances is template reuse for the discovery of issues. In our experience with *OpenfMRI* and *OpenNeuro* (***Markiewicz et al., 2021***), reuse is a top cause for dataset revision after the first release of data. Because of the flexibility and exposure that *TemplateFlow* affords templates and atlases will substantially lower barriers to reuse and feedback reporting, the resource will stimulate the early identification of problems and promote the request of new features to improve available assets.

Inspired by the Conda-forge community repository and the Journal of Open Source Software, the GitHub-based "templateflow" organization is a site for dialogue between members of the neuroimaging community and *TemplateFlow Archive* curators. GitHub issues offer any community member the ability to share their needs with developers and *Archive* curators, for instance by identifying templates or workflow features for potential inclusion in the project. "Pull requests" provide a means for members of the community to directly contribute code or template resources to the *TemplateFlow Archive*.

Decoupling software and templates is indispensable for more reliable and more reproducible study designs

Although there is not yet any standard distance function that can objectively determine whether a template choice is phenotypically proximal to the study's sample, selecting an inappropriate template may introduce so-called "template effects" that bias morphometric analyses and produce incorrect results (***Yoon et al., 2009***). For example, since most generally used templates were created with a sample of adults of European ancestry, a study involving East Asian adults might require a non-default template. More evidently, because of the relative scarcity of nonhuman imaging resources, exposure to template effects is even more pressing in the nonhuman context: e.g., is it appropriate to use a mouse template for the spatial standardization of rat images? Not only are nonhuman templates and atlases fewer, accommodation of such resources in popular software

tools is generally limited. For instance, AFNI (***Cox and Hyde, 1997***) includes a rat template that can be applied in some contexts, while SPM provides functionality only through third-party add-ons (e.g., ***Sawiak et al., 2009***). Second, deviating from software defaults places a knowledge burden on the user. Once the researcher has selected a reference standard space that is suitable for their study population, if their choice is not included by default with the software they plan to use, they must then locate and download the reference template or atlas and integrate it within their analytic pipeline. To our knowledge, only AFNI have made efforts on this direction with their relatively recent `@Install_<template_name>` command, although the tool (i) is not designed to be compatible with other analysis alternatives, and (ii) only provides a minimal set of *TemplateFlow*'s features (i.e., resource download).

On the other hand, for tools like *TemplateFlow* that open up a wide range of options for a given study, the consequently increased methodological flexibility may become a point of concern. ***Carp*** (***2012a***) empirically investigated the consequences of methodological flexibility in neuroimaging, demonstrating that decision points in workflows can lead to substantial variability in analysis outcomes. In a contemporaneous paper, ***Carp*** (***2012b***) contextualized these findings vis-à-vis the inflated risk of false positives, underscoring that analytical variability degrades the reproducibility of studies only *in combination with* (intended or unintended) *selective reporting* of methods and results. Selective reporting, in this particular application, would mean that a researcher explores the results with reference to several templates or atlases and reports only those that confirm the research's hypotheses. *TemplateFlow*'s design accounts for this risk by equipping researchers with the necessary tooling and metadata (unambiguous resource identifiers, versioning and provenance information, querying utilities, etc.) to minimize their reporting burden and ensure completeness. More recently, ***Botvinik-Nezer et al.*** (***2020***) advocated for another approach to the problem of analytical variability: "multiverse" analyses, wherein many combinations of methodological choices are all thoroughly reported and cross-compared when presenting results. Applied to the particular choice of template and atlas combinations, it would thus be desirable to report neuroimaging results with reference to several standard spaces and determine whether the interpretations hold across those references and atlases. *TemplateFlow*'s interoperability empowers users to incorporate this type of analysis into their research by easily making template or atlas substitutions for cross-comparison. For instance, Box 2 shows how *TemplateFlow* works with *fMRIPrep* to automate preprocessing of outputs in multiple standard spaces. This facilitates assessment of the robustness of a result with respect to the template or atlas of choice in accordance with the multiverse approach. ***Botvinik-Nezer et al.*** (***2020***) also promoted pre-registration of studies as a powerful means to fixate methodological choices before the authors have access to intermediate and final results. Here, *TemplateFlow* emerges as a powerful tool to unambiguously document template and atlas choices at pre-registration time.

Discussion

Leveraging our experience developing an open data-sharing platform (OpenNeuro; ***Markiewicz et al., 2021***), BIDS (***Gorgolewski et al., 2016***), and related research instruments such as *MRIQC* (***Esteban et al., 2017***) and *fMRIPrep* (***Esteban et al., 2019***), we propose *TemplateFlow* as a timely resource to bridge gaps in the flexibility and reproducibility of neuroimaging studies. These gaps mostly stem from a software-bound distribution mode of templates and atlases that is the *de facto* standard practice. We argue this practice is oftentimes excessively limiting for researchers (i.e., studying the infant brain or nonhuman brain) if not problematic (i.e., template effects induced by the wrong choice of reference). More worryingly, many scientific communications assume the provenance of templates is completely specified by the choice of software library (e.g., ***Carp, 2012b***). As additional, anecdotal evidence, prompted in part by ***Carp*** (***2012b***), in the Supplementary Materials we show an exploration over 6,048 papers published in the specialized titles *NeuroImage* and *NeuroImage: Clinical* that contained the term "MNI" (for Montreal Neurological Institute; which has

been historically established as *the* standardized space of reference). Our analysis indicates that *MNI space* can refer to any of a family of templates and is not a unique identifier. As a matter of fact, studies carried out with SPM96 (***Friston et al., 2006***) and earlier versions report their results in *MNI space* with reference to the single-subject Colin 27 average template (***Holmes et al., 1998***). However, beginning with SPM99, the software updated its definition of *MNI space* to refer to a new average of 152 subjects linearly aligned (***Mazziotta et al., 1995***). As of SPM12, different modules alternatively use the latter template or a new version created by the MNI in 2009 by means of nonlinear registration (***Fonov et al., 2011***). By contrast, the *MNI template* bundled with FSL was developed by Dr. A. Janke in collaboration with MNI researchers (***Evans et al., 2012***). Although it was generated under the guidance of and using the techniques of the 2006 release of nonlinear MNI templates, this instance is not in fact part of the official portfolio distributed by MNI. Further, FreeSurfer uses a modified version of the "MNI Average Brain (305 MRI) Stereotaxic Registration Model" (a linear MNI template based on 305 subjects; ***Evans et al., 1993***) within some early steps of the `recon-all` pipeline. AFNI has opted for expanding its support to all instances of the *MNI spaces* providing some of the functionalities of *TemplateFlow*. However, utilization and configuration is reserved to expert users, involved tools are not designed for compatibility, and the maintenance burden remains on the shoulders of the package developers. Issues regarding access, unequivocal identification, integration within software workflows, reuse terms, and provenance tracking are only exacerbated when the necessary template or atlas is not a software default.

We address such concerns by promoting a resource based on FAIR Principles. Indeed, it is habitual to find resources in institutional deposits such as the MNI website that lack an explicit usage license (an example at the time of writing[1] is ***Frey et al.*** (***2009***)). Distribution with general-purpose, manually-curated repositories such as NITRC may be more problematic. Beyond the absence of a shared data format because repositories do not mandate any standard, additional problems arise that hinder or block access and reuse. We have found templates at NITRC flagged as available for *freeware noncommercial* use as a general category, but the actual terms for reuse are not accessible. More worryingly, authors may post private resources with the appearance of being open. NITRC's interface allows resources to be nominally released under a permissive open license, but before the data can be accessed, the resource authors require signing a Data Usage Agreement that forbids redistribution[2]. Further details of the advantages of *TemplateFlow* over NITRC for the particular case of template and atlas resource distribution are provided in the Supplementary Table S4. Long term sustainability of the resource is ensured by using minimal cost services (all free at the time of writing) and open source tools.

[1] we have notified the authors and the issue is being resolved

[2] we have shared this instance's URL at NITRC with the reviewers

Limitations

TemplateFlow affords researchers substantial analytical flexibility in the choice of standard spaces of reference. Such flexibility helps researchers minimize "template effects" —by easily inserting the most adequate template— but also opens opportunities for incomplete reporting of experiments. Using *DataLad* or the *TemplateFlow Client*, researchers have at their disposal the necessary tooling for precise reporting: unique identifiers, provenance tracking, version tags, and comprehensive metadata. Therefore, the effectiveness of *TemplateFlow* to mitigate selective reporting is bounded by the user's discretion.

As a research resource, the scope of this manuscript is limited to describing the framework and infrastructure of *TemplateFlow*, highlighting how neuroscientists can leverage this new data archive and the tooling around it. Therefore, some fundamental issues related to this work must be left for future investigation: (i) the overarching problems of cross-template and cross-atlas consistency (***Bohland et al., 2009***); (ii) comparative evaluation of methodological alternatives for producing new templates, atlases and related data; (iii) providing neuroimagers with more objective means to determine the most appropriate template and atlas choices that apply to their research, as well as better understanding "template effects"; (iv) the adequacy of original (MRI, nuclear imaging, etc.) and derived (regularly gridded images, surfaces, etc.) modalities for a specific research

application; or (v) the study of the validity and reliability of inter-template registration, as well as the evaluation of such a component of the *TemplateFlow* framework. However, the proposed framework serves as an ideal keystone to investigate some of the issues above. For instance, the Supplemental Materials describe one of the resource's tools to estimate nonlinear spatial mappings between templates that would be powerful in investigating the issue of consistency (i).

Conclusion

We introduce an open framework for the archiving, maintenance and sharing of neuroimaging templates and atlases called *TemplateFlow* that is implemented under FAIR data sharing principles. We describe the current need for this resource in the domain of neuroimaging, and further discuss the implications of the increased analytical flexibility this tool affords. These two facets of reproducibility —availability (under FAIR guiding principles) of prior knowledge required by the research workflow, and the analytical flexibility such availability affords— are ubiquitous concerns across disciplines. *TemplateFlow*'s approach to addressing both establishes a pattern broadly transferable beyond neuroimaging. We envision *TemplateFlow* as a core research tool undergirding multiverse analyses —assessing whether neuroimaging results are robust across population-wide spatial references— as well as a stepping stone towards the quest of mapping anatomy and function across species.

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Ethical compliance

We complied with all relevant ethical regulations. This resource reused publicly available data derived from studies acquired at many different institutions. Protocols for all of the original studies were approved by the corresponding ethical boards.

Code & data availability statement

All the software components discussed in this paper are available under the Apache 2.0 license, accessible as repositories of https://github.com/templateflow. All templates and associated data are available under corresponding open licenses and accessible as described in the manuscript.

Author contributions

Conceptualization: RC, CJM, KJG, RAP, OE Data curation: RC, EM, OE Topics analysis: RC, RL, OE Funding acquisition: KJG, RAP, OE Methodology: RC, OE Project administration: RAP, OE Resources: YOH, SSG, KJG, RAP, OE Software & Documentation: RC, WHT, MG, EM, CJM, YOH, OE Supervision: RAP, OE Validation: RC, WHT, EM, OE Visualization: RC, RL. Writing – original draft: RC & OE Writing – review & editing: RC, RL, WHT, MG, EM, CJM, YOH, SSG, KJG, RAP, OE.

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Online methods

TemplateFlow comprises four cardinal components: (i) a cloud-based archive, (ii) a Python client for programmatically querying the archive, (iii) automated systems for synchronizing and updating archive data, and (iv) inter-template registration workflows. Here, we discuss the details of each component's implementation in turn, as well as the manner in which they interact with one another to form a cohesive whole.

The *TemplateFlow Archive*.

The archive itself comprises directories of template data in cloud storage. For redundancy, the data are stored on both Google Cloud using the Open Science Framework (OSF) and on Amazon's Simple Storage Service (S3). Prior to storage, all template data must be named and organized in directories conforming to a data structure adapted from the Brain Imaging Data Structure (BIDS) standard (***Gorgolewski et al., 2016***). The precise implementation of this data structure is a living document and is detailed on the *TemplateFlow* homepage (http://www.templateflow.org). We detail several critical features here.

The archive is organized hierarchically, and descriptive metadata follow a principle of inheritance: any metadata that apply to a particular level of the archive also apply to all deeper levels. At the top level of the hierarchy are directories corresponding to each archived template. If applicable, within each template directory are directories corresponding to sub-cohort templates. Names of directories and resource files constitute a hierarchically ordered series of key-value pairs terminated by a suffix denoting the datatype. For instance, `tpl-MNIPediatricAsym_cohort-3_res-high_T1w.nii.gz` denotes a T1-weighted template image file for resolution "high" of cohort "3" in the "MNIPediatricAsym" template (where the definitions of each resolution and cohort are specified in the template metadata file, *TemplateFlow Archive*). The most common *TemplateFlow* datatypes are indexed in Suppl. Table S2; an exhaustive list is available in the most current version of the BIDS standard (https://bids.neuroimaging.io/).

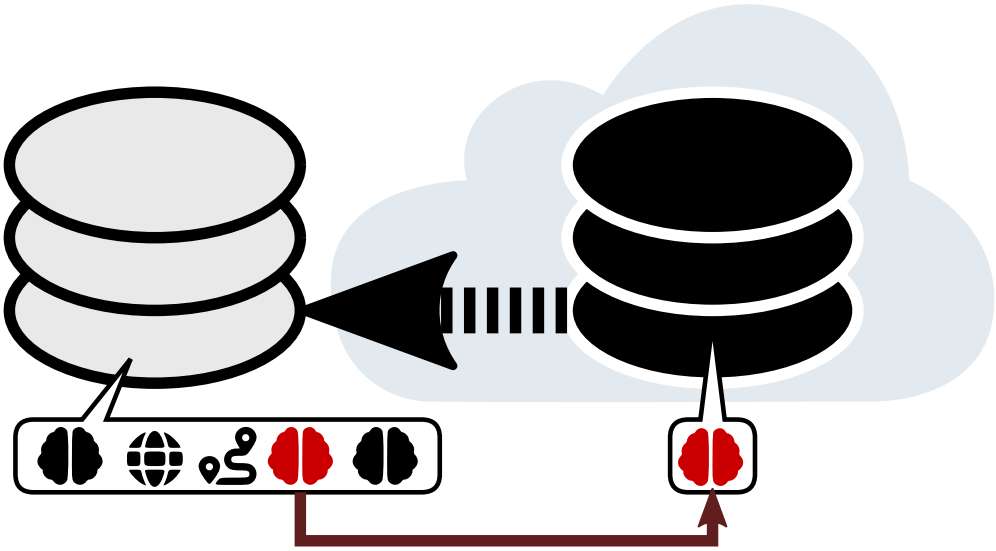
Within each directory, template resources include image data, atlas and template metadata, transform files, licenses, and curation scripts. All image data are stored in gzipped NIfTI-1 format and are conformed to RAS+ orientation (i.e., left-to-right, posterior-to-anterior, inferior-to-superior, with the affine qform and sform matrices corresponding to a cardinal basis scaled to the resolution of the image). Template metadata are stored in a JavaScript Object Notation (JSON) file called `template_description.json`; an overview of metadata specifications is provided in Figure 3 of the main manuscript. In brief, template metadata files contain general template metadata (e.g., authors and curators, references), cohort-specific metadata (e.g., ages of subjects included in each cohort), and resolution-specific metadata (e.g., dimensions of images associated with each resolution). Atlas metadata are often stored in TSV format and specify the region name corresponding to each atlas label. Transform files are stored in HDF5 format and are generated as a diffeomorphic composition of ITK-formatted transforms mapping between each pair of templates.

The archive has a number of client-facing access points to facilitate browsing of resources. Key among these is the archive browser on the *TemplateFlow* homepage, which indexes all archived resources and provides a means for researchers to take inventory of possible templates to use for their study.

The Python client.

TemplateFlow is distributed with a Python client that can submit queries to the archive and download any resources as they are requested by a user or program. Valid query options correspond approximately to BIDS key-value pairs and datatypes. A compendium of common query arguments is provided in Suppl. Table S2, and comprehensive documentation is available on the *TemplateFlow* homepage.

When a query is submitted to the *TemplateFlow* client, the client begins by identifying any files in the archive that match the query. To do so, it uses *PyBIDS* (***Yarkoni et al., 2019***), which exploits



```
>>> from templateflow import api as tflow
>>> tflow.get('MNI152NLin6Asym', desc=None, resolution=1,
...           suffix='T1w', extension='nii.gz')
PosixPath('/templateflow_home/tpl-MNI152NLin6Asym/tpl-
          MNI152NLin6Asym_res-01_T1w.nii.gz')
```

Figure 4. Example usage of the Python-based *TemplateFlow Client*. After importing the API, the user submits a query for the T1-weighted FSL version of the MNI template at 1 mm resolution. The client first filters through the archive, identifies any files that match the query, and finds their counterparts in cloud storage. It then downloads the requested files and returns their paths in the local *TemplateFlow* installation directory. Future queries for the same resource can be completed without any re-downloading.

the BIDS-like architecture of the *TemplateFlow Archive* to efficiently scan all directories and filter any matching files. Next, the client assesses whether queried files exist as data in local storage. When a user locally installs *TemplateFlow*, the local installation initially contains only lightweight pointers to files in OSF cloud storage. These pointers are implemented using *DataLad* (***Halchenko et al., 2021***), a data management tool that extends git and git-annex. *TemplateFlow* uses *DataLad* principally to synchronize datasets across machines and to perform version control by tracking updates made to a dataset.

If the queried files are not yet synchronized locally (i.e., they exist only as pointers to their counterparts in the cloud), the client instructs *DataLad* to retrieve them from cloud storage. In the event that *DataLad* fails or returns an error, the client falls back on redundancy in storage and downloads the file directly from Amazon's S3. When the client is next queried for the same file, it will detect that the file has already been cached in the local filesystem. The use of resource pointers with the client thus enables lazy loading of template resources. Finally, the client confirms that the file has been downloaded successfully. If the client detects a successful download, it returns the result of the query; in the event that it detects a synchronization failure, it displays a warning for each queried file that encountered a failure.

Continued functionality and operability of the client is ensured through an emphasis on maximizing code coverage with unit tests. Updating the client requires successful completion of all unit tests, which are automatically executed by continuous integration (CI) and continuous delivery (CD) services connected to GitHub. CI and CD also keep the web-based archive browser up to date by automatically indexing data files.

Ancillary and managerial systems.

TemplateFlow includes a number of additional systems and programs that serve to automate stages of the archive update process, for instance addition of a new template or revision of current template resources. To facilitate the update and extension process, *TemplateFlow* uses GitHub actions to automatically synchronize dataset information so that all references remain up-to-date with the

Box 2. Integration of *TemplateFlow* in processing workflows

TemplateFlow maximizes the accessibility and reuse potential of templates and atlases. For example, let's reuse the base configuration file for FSL FEAT we proposed in our paper (***Esteban et al., 2019***). The design file `design.fsf` specifies a simple preprocessing workflow with FSL tools. The simplified code listing below shows that, just to make non-default templates available to FSL using the graphical user interface (GUI), at least five steps are necessary:

```
# 1. User determines two nondefault templates they want to spatially normalize into
# 2. User manually downloads templates, extracts the required files from packages
$ curl -sSL <url> | tar zxv --no-same-owner -C /data/templates/
# 3. User opens FSL's GUI, edits the target template box content pointing to the appropriate files
# 4. User generates FSL configuration files to permit batch execution on the command line
# 5. For the default and the two nondefault templates, execute FSL's feat:
$ feat design_<template>.fsf
```

The outputs of each `feat design_<template>.fsf` call will follow the pre-specified patterns of FSL, with whatever customization the user has introduced into the design file. The user, therefore, must then adapt the downstream analysis tools to correctly interpret the derived dataset, in each standard space, or reformat the output dataset according to the expectations of the analysis tools.
The user is also responsible for all aspects of provenance tracking and adequately reporting them in their communications. Information such as version of the template (or download date), citations to relevant papers, and other metadata (e.g., RRIDs) must be accounted for manually throughout the research process.

In contrast, tools using *TemplateFlow* dramatically simplify the whole process (note that `MNI152NLin2009cAsym` and `OASIS30Ants` are the two templates not found within the FSL distribution, and `MNI152NLin6Asym` denotes *FSL's MNI space* (i.e., the default FSL template):

```
$ fmriprep /data /derivatives participant --output-spaces MNI152NLin2009cAsym MNI152NLin6Asym OASIS30Ants
```

fMRIPrep generates the results with BIDS-Derivatives organization for the three templates. The tool also leverages *TemplateFlow* to generate a *boilerplate citation text* that includes the full names, versions and references to credit the template's authors for each of the templates involved.
fMRIPrep internally stages one spatial normalization workflow for each of the output spaces. Each of these normalization sub-workflows uses a simple line of Python code to retrieve the necessary resources from *TemplateFlow* using the *TemplateFlow Client* interface (Figure 4):

```
>>> from templateflow.api import get
>>> tpl_ref_file = get("MNI152NLin6Asym", desc=None, resolution=1, suffix="T1w", extension="nii.gz")
```

One detail overseen in the FSL example is that, for a robust spatial normalization process, a precise binary mask of the brain is generally used. While FSL would require the user to manually set this mask up in the GUI, in the case of *TemplateFlow*, it requires a second minimal call:

```
>>> msk_ref_file = get("MNI152NLin6Asym", desc="brain", resolution=1, suffix="mask", extension="nii.gz")
```

These examples are extreme simplifications of what a pipeline developer can automate and make more robust by integrating *TemplateFlow* in their workflows.
For further examples on how *TemplateFlow* can be leveraged, *PyNets* is a package for ensemble learning of functional and structural connectomes (***Pisner and Hammonds, 2020***), and *NetPlotBrain* for visualization (***Thompson and Fanton, 2021***).

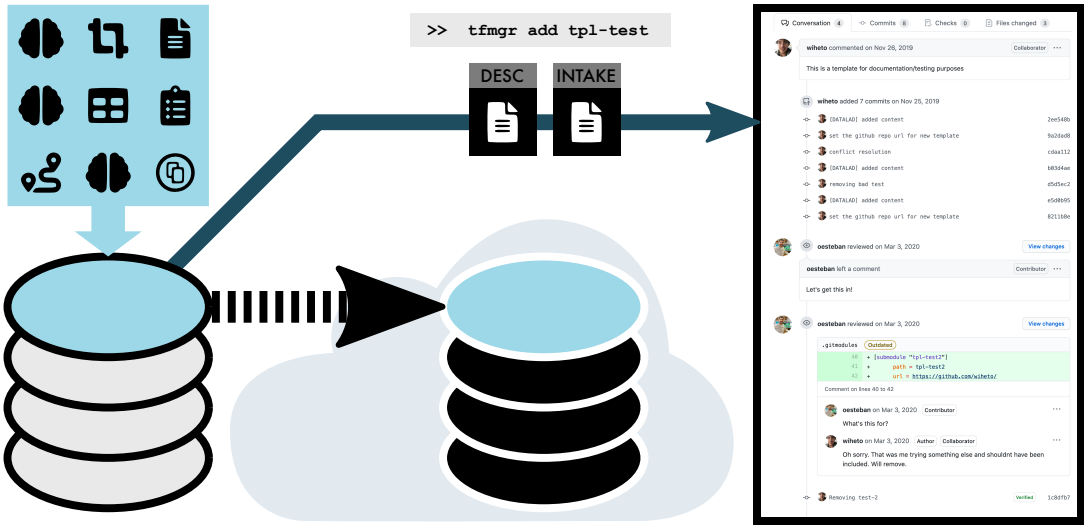


Figure 5. Contributing a new resource with the *TemplateFlow Manager*. To contribute a new template to *TemplateFlow*, members of the community first organize template resources to conform to the BIDS-like *TemplateFlow* structure. Next, `tfmgr` (the *TemplateFlow Manager*, see Suppl. Table S3) synchronizes the resources to OSF cloud storage and opens a new pull request proposing the addition of the new template. A subsequent peer-review process ensures that all data are conformant with the *TemplateFlow* standardd. Finally, *TemplateFlow* curators merge the pull request, thereby adding the template into the archive.

current dataset. These actions are triggered whenever a pull request to *TemplateFlow* is accepted. For example, GitHub actions are used to update the browser of the *TemplateFlow Archive* so that it displays all template resources as they are uploaded to the archive.

Whereas the *TemplateFlow Client* synchronizes data from cloud storage to the local filesystem, a complementary *TemplateFlow Manager* handles the automated synchronization of data from the local filesystem to cloud storage. The Python-based manager is also used for template intake, i.e., to propose the addition of new templates to the archive. To propose adding a new template, a user first runs the *TemplateFlow Manager* using the `tfmgr add <template_id> --osf-project <project_id>` command.

The manager begins by using the *TemplateFlow* client to query the archive and verify that the proposed template does not already exist. After verifying that the proposed template is new, the manager synchronizes all specified template resources to OSF cloud storage. It then creates a fork of the `tpl-intake` branch of the *TemplateFlow* GitHub repository and generates an intake file in Tom's Obvious Minimal Language (TOML) markup format; this intake file contains a reference to the OSF project where the manager has stored template resources. The *TemplateFlow Manager* commits the TOML intake file to the fork and pushes to the user's GitHub account. Finally, it retrieves template metadata from `template_description.json` and uses the metadata to compose a pull request on the `tpl-intake` branch. This pull request provides a venue for discussion and vetting of the proposed addition of a new template.