

# EBRAINS Data Descriptor

## TITLE

Parcellation-based structural and resting-state functional brain connectomes of a healthy cohort (v1.1)

## AUTHORS

Justin W. M. Domhof<sup>1,2</sup>, Kyesam Jung<sup>1,2</sup>, Simon B. Eickhoff<sup>1,2</sup>, Oleksandr V. Popovych<sup>1,2</sup>

## AFFILIATIONS

1. Institute of Neuroscience and Medicine, Brain and Behaviour (INM-7), Research Centre Jülich, Jülich, Germany

2. Institute for Systems Neuroscience, Medical Faculty, Heinrich Heine University Düsseldorf, Düsseldorf, Germany

**corresponding author(s):** Justin Domhof (j.domhof@fz-juelich.de), Oleksandr Popovych (o.popovych@fz-juelich.de)

## ABSTRACT

Nowadays, the connectivity patterns in brain networks are of special interest, as they may reflect the communication in the brain at the structural and functional levels. Their extraction, however, is a complex process that requires a deep knowledge of the magnetic resonance imaging (MRI) data processing methods. Furthermore, there is no consensus as to which parcellation of the brain is most suitable for a given analysis. Therefore, in this dataset 20 different state-of-the-art brain parcellations were used to reconstruct the region-based empirical structural connectivity (representing the anatomical axonal tracts) and functional connectivity (representing the temporal correlation between neuronal activity of brain regions) from diffusion-weighted (dwMRI) and resting-state functional magnetic resonance imaging (fMRI) data, respectively. The repository provides individual connectomes for 200 subjects from the Human Connectome Project. The data can be used by members of the neuroimaging community to investigate the structural and functional human connectomes, and to extend the investigation to the whole-brain models for further analyses of the brain structure and function.

## METHODS

The empirical connectomes included in this study were reconstructed for 200 unrelated, healthy young adults (96 males) from the S1200 Young Adult Open Access dataset of the Human Connectome Project (HCP) (D. C. Van Essen et al., 2012; David C. Van Essen et al., 2013). Therefore, the data use terms of the HCP dataset are also applicable when using the data included in this repository, see <https://www.humanconnectome.org/study/hcp-young-adult/document/wu-minn-hcp-consortium-open-access-data-use-terms> for details. Here, we separately discuss the reconstruction of the structural connectivity (SC) and functional connectivity (FC) from the diffusion-weighted and functional magnetic resonance imaging data (dwMRI and fMRI, respectively) included in the mentioned HCP dataset. Afterwards, we present the 20 different state-of-the-art brain parcellations for which we extracted the

region-based connectomes. The code used to acquire our results is available elsewhere (<https://jugit.fz-juelich.de/inm7/parcellation-modelling>).

#### *SC reconstruction from dw-MRI data*

We used a workflow developed in-house to reconstruct the SC from diffusion-weighted magnetic resonance imaging data, see [https://github.com/inm7/vbc\\_dwmri](https://github.com/inm7/vbc_dwmri). This workflow consisted of four stages: (1) preprocessing of the diffusion-weighted images, (2) computing the whole-brain tractography, (3) transformation of the atlas images to the subject's native space, and finally (4) reconstruction of the SC matrices. The pipeline can be regarded as a wrapper of functions included in the ANTs (Tustison et al., 2010), FreeSurfer (Dale et al., 1999), FSL (Jenkinson et al., 2012) and MRtrix3 (J-Donald Tournier et al., 2019) software packages. Computations were performed on the JURECA high-performance computing cluster (Jülich Supercomputing Centre, 2018).

When preprocessing the images, FreeSurfer functions were used to perform bias field correction, tissue segmentation, cortical (surface) reconstruction, volume-surface conversion and surface deformation on the T1-weighted images of the subjects. FreeSurfer functions were also used to perform head motion and eddy current distortion correction on the diffusion-weighted images, whereas MRtrix3 functions denoised them and performed bias field correction. The diffusion-weighted images were registered to the T1-weighted images by the linear and nonlinear transformation functions of FSL. Afterwards, tissue segmentation was also performed for the diffusion-weighted images. (2) Subsequently, the whole-brain tractography was computed on the basis of the diffusion-weighted images by using MRtrix3 functions. The response functions for spherical deconvolution were estimated using a multi-shell-multi-tissue constrained algorithm (Jeurissen et al., 2014). Through these response functions, the fibre-oriented distributions could be determined from the diffusion-weighted images. The whole-brain tractography was completed via a second-order integration over these distributions by means of a probabilistic algorithm (Jacques-Donald Tournier et al., 2010). We used the following tracking parameter settings: number of streamlines = 10M, step size = 0.625 mm, angle = 45°, min. length = 2.5 mm, max. length = 250 mm, FOD amplitude for terminating tract = 0.06, max. attempts per seed = 50, max. number of sampling trials = 1000 and down-sampling = 3 mm. (3) FSL function were used to linearly and nonlinearly transform the brain atlas images from the standard space to the subject's native space. (4) Eventually, the MRtrix3 function `tck2connectome` was used to derive the number of streamlines and their average length for all pairs of parcels included in a particular parcellation.

#### *Derivation of the FC from fMRI data*

Blood oxygen level dependent (BOLD) signals were extracted from the ICA-FIX denoised resting-state fMRI data as provided by the Human Connectome Project (Griffanti et al., 2014). Here, the mean BOLD intensity averaged across all voxels in each parcel included in the considered parcellation scheme was calculated per brain volume. The result comprised one signal time series per parcel. Individual time series were linearly detrended and z-scored. The FC matrix was subsequently reconstructed by taking the Pearson correlation coefficients across the time series for all pairs of parcels. The original data provided 4 resting-state sessions for all subjects (2 phase encoding directions scanned on 2 days). Therefore, we calculated 4 different FC matrices corresponding to each of these sessions. In addition, we calculated the FC associated with the concatenated time series; this FC can be regarded as the average FC of the subject.

#### *Brain parcellations*

The SC and FC of each subject were reconstructed on the basis of the 20 different brain atlases (or parcellations) included in Table 1. The used brain atlases are available for download provided by the

corresponding publications cited in Table 1. The links for download are collected in the files “Link.txt” included in the repository. In order to enhance the comparability between atlases, we modified the original atlas images so that they only covered the cerebral cortex (except for the Julich-Brain atlas, see Table 1) and were sampled to the MNI152 nonlinear template space (Grabner et al., 2006). The details of these modifications vary across parcellations. We, therefore, have added the scripts performing their modifications to the repository.

These atlases were selected in order to balance between parcellations derived from functional data (Craddock et al. (2012), Shen et al. (2013), Schaefer et al. (2018) and Urchs et al. (2019)) and structural information, comprising the other brain atlases shown in Table 1. Note, however, that the Julich-Brain atlas was not included in the first version of the repository (Domhof et al., 2021) that was used in the modeling study (Domhof et al., 2021a), but was added in the current version. In addition, the considered parcellations were constructed via a variety of methodologies including boundary detection algorithms, histological stainings and diverse clustering approaches. This diversity in brain parcellation compilation paradigms enhanced the probability of finding parcellation-induced deviations. When available, we also included parcellations constructed through the same method in multiple granularities so that the effect of this quantity can be investigated as well.

**Table 1.** Overview of the used brain parcellation schemes with the number of parcels after atlas image modifications and associated publications.

Atlas name	Parcels	References
MIST	31	(Urchs et al., 2019)
	56	
	103	
	167	
	38	
Craddock	56	(Craddock et al., 2012)
	108	
	160	
Shen 2013	79	(Shen et al., 2013)
	156	
Schaefer	100	(Schaefer et al., 2018)
	200	
Harvard-Oxford	48	(Desikan et al., 2006; Frazier et al., 2005; Goldstein et al., 2007; Makris et al., 2006)
	96	
Desikan-Killiany	70	(Desikan et al., 2006)
von Economo-Koskinas	86	(Scholtens et al., 2018; von Economo & Koskinas, 1925)
AAL (version 2)	92	(Rolls et al., 2015; Tzourio-Mazoyer et al., 2002)
Destrieux	150	(Destrieux et al., 2010)
Brainnetome	210	(Fan et al., 2016)
Julich-Brain (version 2.9)	294	(Amunts et al., 2020; Amunts et al., 2021)

## TECHNICAL VALIDATION

The technical quality of the connectomes included in this repository highly depends on the quality of the neuroimaging data included in the S1200 Young Adult Open Access dataset. This quality has been assured by the Human Connectome Project. No ground truth exists for the SC and the FC. This is especially applicable to the FC derived from the resting-state fMRI data, where no references can be found to the observed dynamics as compared to, for example, the task-evoked activity. Still, for the reconstruction of both types of connectomes, we wielded approaches and software packages that are extensively tested

and widely used. In particular, the preprocessing of the data was in line with published recommendations (Glasser et al., 2013; Salimi-Khorshidi et al., 2014; J-Donald Tournier et al., 2019). This enhanced the quality and reliability of the presented connectivity matrices. Additionally, our workflow used the freely available software packages of FSL (Jenkinson et al., 2012), FreeSurfer (Dale et al., 1999), ANTs (Tustison et al., 2010) and MRtrix3 (J-Donald Tournier et al., 2019), which process the magnetic resonance imaging data with high quality. Finally, the Pearson correlation coefficients across the BOLD time series were calculated by the standard NumPy module for Python (Walt et al., 2011). These procedures and tools have contributed to the quality and reliability of the connectomes included in this repository.

## USAGE NOTES

As mentioned above, the connectivity matrices included in this repository comprise the individual SC and FC of 200 subjects for 20 different parcellations. The data are included as text files and hence can be processed by many different programming languages and software packages for further analyses. Examples of such analyses include atlas-induced variations in the structure-function relationship of individual subjects as estimated through diverging paradigms. Different methodologies include, but are not limited to, the statistical analysis of structure-function dependencies and dynamical whole-brain models (Suárez et al., 2020). In the latter paradigm, a network model is built on the basis of the SC, whereas the FC can be used to validate how well simulations of the constructed model replicate resting-state dynamics (Honey et al., 2009; Popovych et al., 2019). In particular, the presented data not only enable the investigation of atlas-induced group differences, but also parcellation-specific intersubject variabilities.

## SPATIAL ANCHORING:

All brain atlas images and the used MRI data were sampled in the volumetric MNI152 standard space included in FSL (MNI152 nonlinear 6<sup>th</sup> generation, see also <https://fsl.fmrib.ox.ac.uk/fsl/fslwiki/Atlases>). In addition, we ensured the parcellations only covered the cerebral cortex (except for the Julich-Brain atlas). We included the atlas image modification scripts as well so that the user can check the performed procedure. We also provided a summary of the processing steps in the form of a markdown file for each parcellation considered.

## DATA RECORDS

In the repository, the data are stored in the following directory structure:

```
... repository-root/
..... EBRAINS-DataDescriptor_AtlasBasedHCPconnect_SC-FC_v1.1.pdf [This data description file]
..... <Atlas name>/
..... 0ImageProcessing/
..... Link.txt [Text file with the link to the original parcellation images]
..... Modifications.md [Markdown file with the summary of the processing steps]
..... Modifications.sh [Shell script used to process the atlas images]
..... 1StructuralConnectivity/
..... <Subject ID>/
..... Counts.csv [File with the streamline counts matrix]
..... Lengths.csv [File with the average streamline lengths matrix]
..... 2FunctionalConnectivity/
..... <Subject ID>/
```

..... **EmpCorrFC\_<session>.csv** [File with the FC of an individual session]

..... **EmpCorrFC\_concatenated.csv** [File with the FC of the concatenated time series]

The folders in the root directory are named after the atlas used to reconstruct the SC and FC. Each atlas folder is zipped. This name follows the format:

**<Number of parcels>-<Name of the atlas>.**

The data of the atlases are all organised in the same data structure. The folder named **0ImageProcessing** holds three files. **Link.txt** is a text file containing the information on how to obtain the original parcellation images. The **Modifications.md** file is a Markdown file and contains an explanation of the atlas image processing steps. The other file **Modifications.sh** (**Modifications.py** for the Julich-Brain atlas) is a shell (python) script that actually performed the necessary image processing. It can be run in a Unix environment, and requires that FreeSurfer (Dale et al., 1999) and FSL (Jenkinson et al., 2012) are installed on the system.

The **1StructuralConnectivity** and **2FunctionalConnectivity** folders hold a number of subfolders that each correspond to a particular subject, and contain the actual connectomes in a text format. Each connectome file contains data with dimensions  $N \times N$  ( $N$  being the number of parcels). **Counts.csv** and **Lengths.csv** contain the streamline counts between the brain regions included in the parcellation and their average lengths, respectively. **EmpCorrFC\_<session>.csv** is the FC matrix corresponding to a particular resting-state session. Here, **<session>** can either be **REST1-LR**, **REST1-RL**, **REST2-LR** or **REST2-RL**. Finally, **EmpCorrFC\_concatenated.csv** includes the FC matrix calculated on the basis of the concatenated time series.

## CODE AVAILABILITY

The code used for the acquisition of these data are stored in an external git repository hosted at Forschungszentrum Jülich (<https://jugit.fz-juelich.de/inm7/parcellation-modelling>). FreeSurfer (Dale et al., 1999), FSL (Jenkinson et al., 2012), ANTs (Tustison et al., 2010), MRtrix3 (J-Donald Tournier et al., 2019) and Python version 3 (Python Software Foundation, <https://www.python.org/>) are required to be installed on the system in order to run the software. The source code has been successfully tested on multiple Unix systems.

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## Author contributions

S.B.E., O.V.P. and J.W.M.D. conceived the study; K.J. performed the whole-brain tractography calculations; J.W.M.D. calculated the SC and FC data; O.V.P. contributed to technical validation and supervised the study; J.W.M.D. and O.V.P. both drafted the manuscript. All authors were involved in the preparation of the manuscript.

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