Supplementary Data

Gap and Silhouette Methods for Determining Number of Clusters

The determination is made from the Gap method by the following:

1. Cluster the observed data, varying the number of clusters from $k = 1, ..., kmax$, and compute the corresponding total within intracluster variation Wk.
2. Generate B reference data sets with a random uniform distribution. Cluster each of these reference data sets with varying number of clusters $k = 1, ..., kmax$, and compute the corresponding total within intracluster variation Wkb.
3. Compute the estimated gap statistics as the deviation of the observed Wk value from its expected value Wkb under the null hypothesis: $\text{Gap}(k) = 1\text{B}\Sigma b = 1\text{Blog}(W^*kb) - \log(Wk)\text{Gap}(k) = 1\text{B}\Sigma b = 1\text{Blog}(Wkb^*) - \log(Wk)$. Compute also the standard deviation of the statistics.
4. Choose the number of clusters as the smallest value of k such that the gap statistics is within one standard deviation of the gap at $k + 1$: $\text{Gap}(k) \geq \text{Gap}(k + 1) - s_{k+1}$.

And for the Silhouette method by the following:

1. Compute clustering algorithm (e.g., k-means clustering) for different values of k. For instance, by varying k from 1 to 10 clusters.
2. For each k, calculate the average silhouette of observations.
3. Plot the curve according to the number of clusters k.

4. The location of the maximum is considered the appropriate number of clusters.

These methods are programmed into the GIFT software, which outputs the estimated optimal number of clusters, and a plot (see example below, Supplementary Fig. S1). We note there is no definitive answer to this question. The optimal number of clusters is always somewhat subjective and depends both on the method used for measuring similarities and the parameters used for partitioning. However, in this instance, both methods used (Gap and Silhouette) agreed on the optimal number of clusters. Because of this limitation, we returned to the analysis and reran with two clusters and found results consistent with that reported in the article (e.g., fMRI showed differences between healthy controls [HC] and schizophrenia patients [SP] in dwell time, but no significant metastate statistics differences).

Window Size and MEG Data

We examined a variety of window lengths and found that the results are similar in structure; however, we lose high-frequency information as we decrease the window size, while results appear to become washed out with longer window sizes for some cluster states (Supplementary Figs. S2, S3).

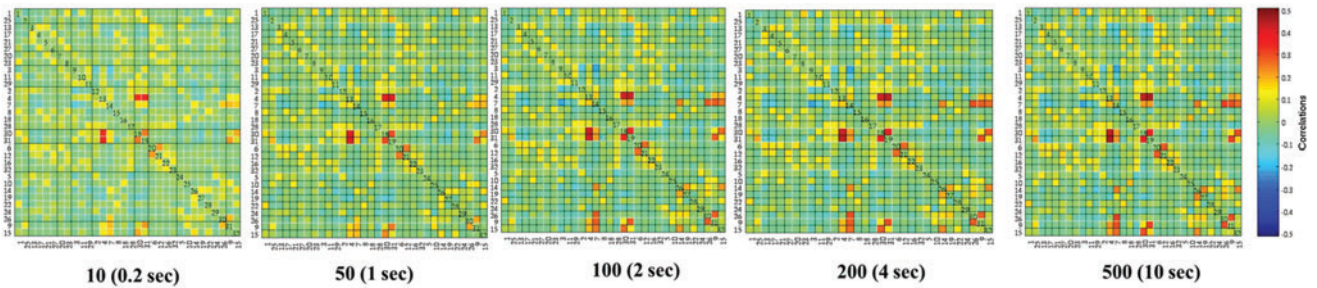## Distribution of Metastate Statistics Between HC and SP Groups

The kernel density is estimated with MATLAB's ksdensity function, which uses an optimal Gaussian kernel (Supplementary Figs. S4, S5).
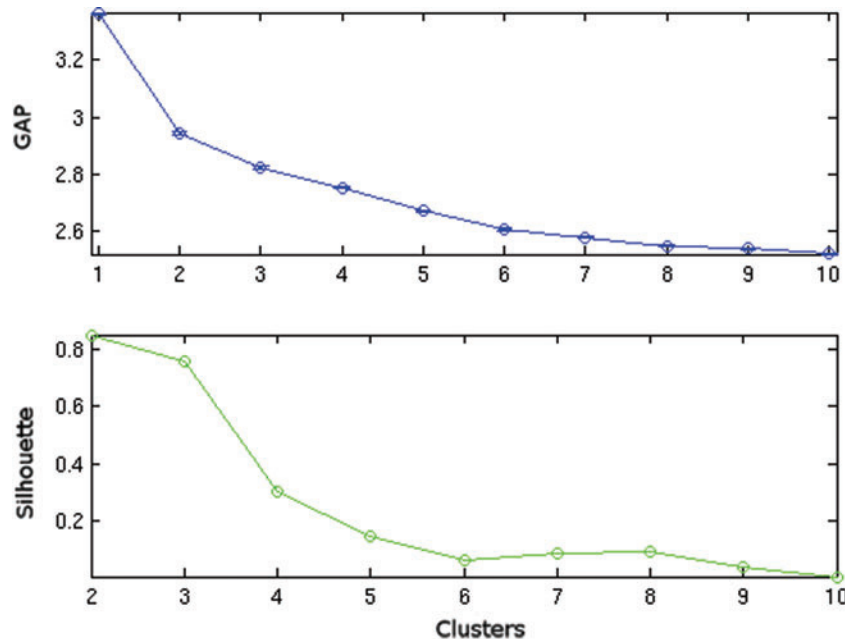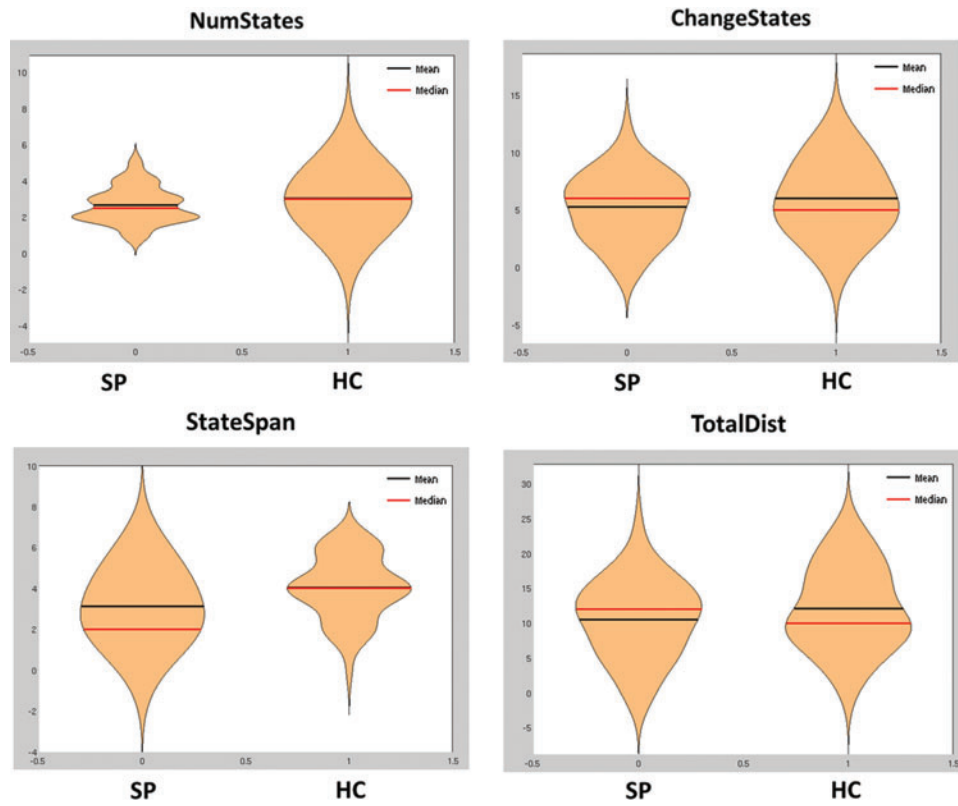

SUPPLEMENTARY FIG. S1. Plot of Gap and Silhouette methods' determination of optimal number of clusters for magnetoencephalography (MEG) data.
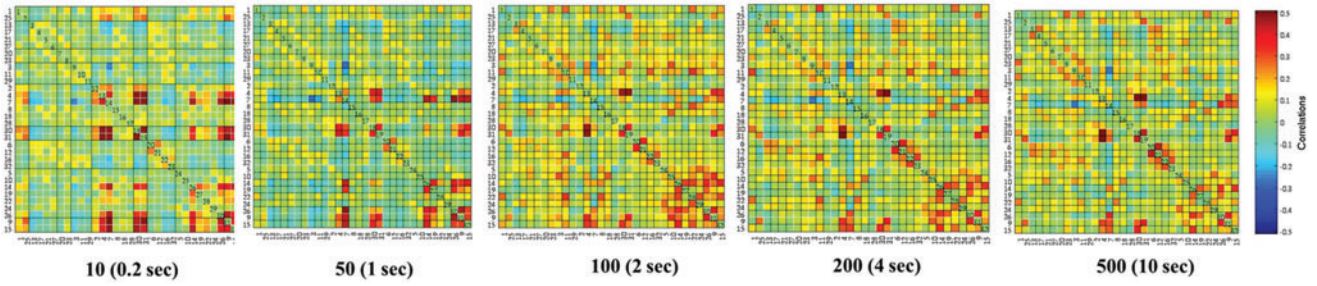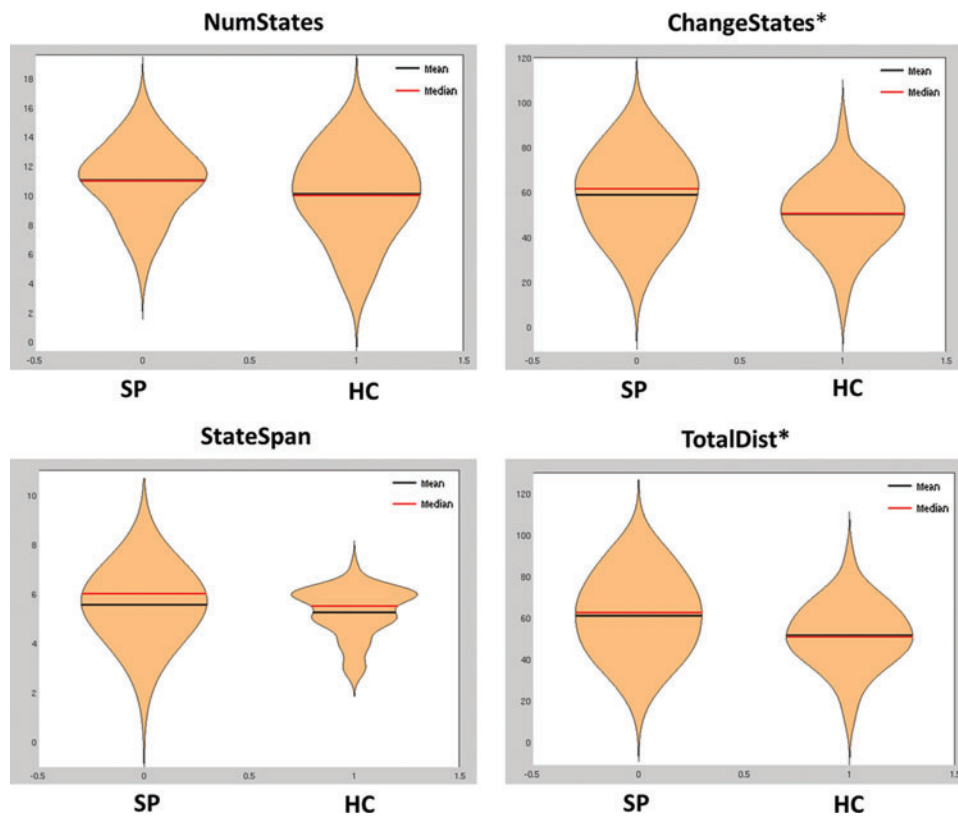
SUPPLEMENTARY FIG. S2. Example of how window length changes results for a highly connected MEG cluster state.

SUPPLEMENTARY FIG. S3. Example where there appears to be less effect of window size on the cluster state.

SUPPLEMENTARY FIG. S4. Distribution of metastate statistics between HC and SP groups for fMRI data.

SUPPLEMENTARY FIG. S5. Distribution of metastate statistics between HC and SP groups for MEG data. *Indicates where we have reported significant differences between SP and HC groups.