## *Supplementary methods*

## Center of rotation

It might seem intuitive to calculate the translation from |**t**|, the displacement of $c_S$, the center of mass of S. However, except for translation parallel to **u**, **t** may arise from rotation about a physically meaningful axis that does not pass through $c_S$. We define an axis as physically meaningful if this axis passes near the interface between L and S, that is, the residues that define the 6 Å contacts between L and S. We define an axis as passing near a set of residues if the $C_\alpha$ atom of any residue in the set is no more than 5.0 Å from the axis. To assess this, we first find a center of rotation $c_R$, such that the motion can be described as a rotation by $\theta$ about **u**, centered at $c_R$, and a translation $T_u$ parallel to **u**.

To do this, we first find the basis vectors $\mathbf{e_x}$, $\mathbf{e_y}$, and $\mathbf{e_z}$ of a right-handed orthogonal coordinate system centered at $c_R$ describing the counterclockwise motion from state A to state B. Let $s_1$ and $s_2$ be the centers of $S_A$ and $S'_B$, and let **s** be the vector between the two centers. Let $\mathbf{e_z} = \mathbf{u}$, and let $\mathbf{e_x}$ lie in a plane defined by $\mathbf{e_z}$ and the midpoint of **s** such that $s_1$ and $s_2$ are in the ($\mathbf{e_x}$,- $\mathbf{e_y}$) and ($\mathbf{e_x}$, $\mathbf{e_y}$) quadrants, respectively. Then, $\mathbf{e_x} = \text{unit}(\mathbf{s} \times \mathbf{e}_z)$, where $\text{unit}(\mathbf{v}) = \mathbf{v}/|\mathbf{v}|$, and $\mathbf{e_y} = \mathbf{e}_z \times \mathbf{x}$.

Then, we find the distance of $s_1$ from the origin in the $\mathbf{e_y}$ and $\mathbf{e_x}$ directions. Since $\mathbf{e_x}$ lies in a plane bisecting **s**, $s_1$ is $y = \frac{1}{2}(\mathbf{s} \bullet \mathbf{e_y})$ from the origin in the $-\mathbf{e_y}$ direction. Next, we triangulate to find $x$, the distance of $s_1$ from the origin in the $\mathbf{e_x}$ direction:

$$x = \frac{y}{\tan(\frac{1}{2}\theta)}.$$

To find $c_R$, we simply extrapolate back:

$$c_R = s_1 - x\mathbf{e_x} + y\mathbf{e_y}.$$