S3 Text. Structural similarity score for model clustering.

The $S_{\text{mirror}}$ score of a given pair of models $i$ and $j$ is computed as:

$$S_{\text{mirror},i,j} = Eqv_{i,j} \times \frac{dRMSD_n}{\max(dRMSD)} \times \frac{\text{max}(dRMSD)}{RMSD_n}$$

Where $Eqv_{i,j}$ is the number of equivalent positions between two superimposed structures within a specific distance cut-off; $dRMSD_n$ is the normalized (i.e., the dRMSD divided by the maximal dRMSD in all structural comparisons) distance RMSD between two aligned structures; and $RMSD_n$ is the normalized RMSD between two aligned structures. This results in a comparison matrix, consisting of all-against-all $S_{\text{mirror}}$ scores, which is then used to resolve structural mirrors (conformations with the same IMP objective function that are mirrors of each other). Next, the comparison matrix is input to the