

### **S3 Text. Structural similarity score for model clustering.**

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

$$S_{mirror_{i,j}} = Eqv_{i,j} \times \frac{dRMSD_n / \max(dRMSD)}{RMSD_n / \max(RMSD)}$$

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  $S_{mirror}$  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