

## Supplementary data II.

Figure S2 presents results of grid search performed for optimising the quadruplet required to define flexibility classes. Each quadruplet was scored according to the selection criteria defined in Methods section 2.9. For clarity, are represented the different maps for each pair of parameters even if the search is performed for the four parameters. The scores are represented by colour scale from dark blue for low score to dark brown to high scores. The quadruplet  $(-1.5, -0.5, 2.2, 1.1)$  obtaining the score of 9 (dark brown) is finally selected.

