Supplemental Information - Resolving the Fine Structure in the EnergyLandscapes of Repeat Proteins

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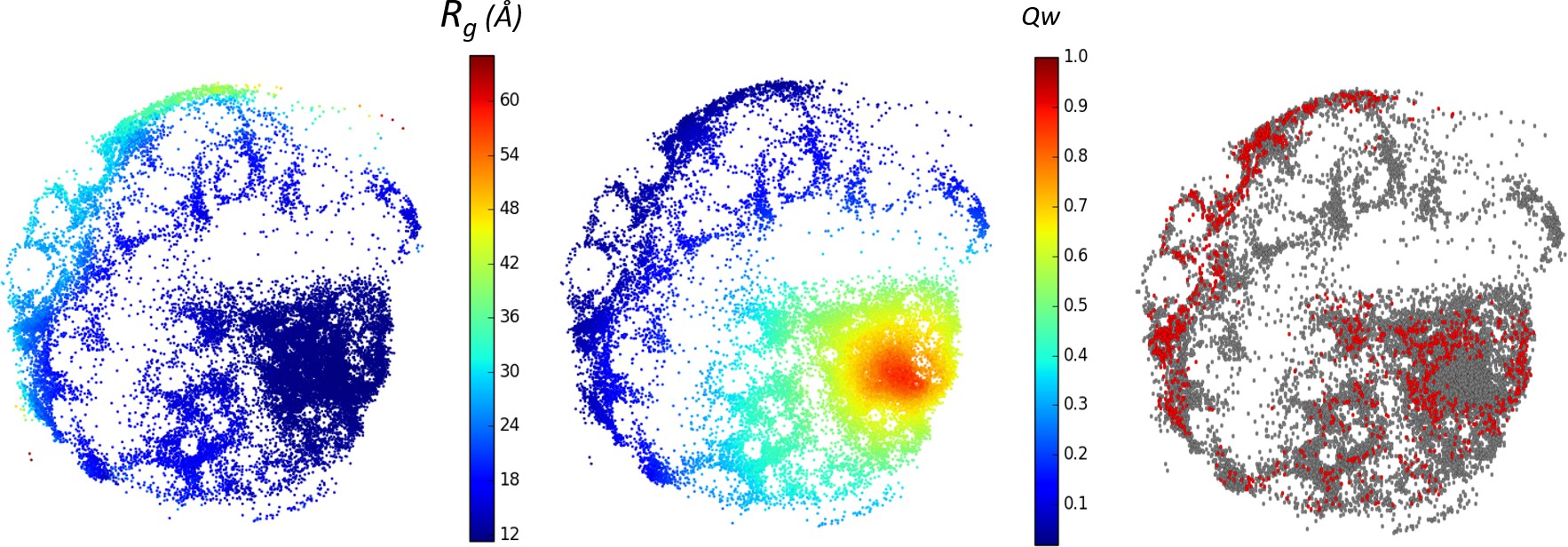


Figure S1: ELViM 2D projection of the conformational phase space of 3ANK as (A) a func- tion of the radius of gyration and (b) a function of *Qw* coordinate. (C) Projection showing the conformations obtained with two different simulations: the unbiased conformations in red, and the biased conformations in grey.

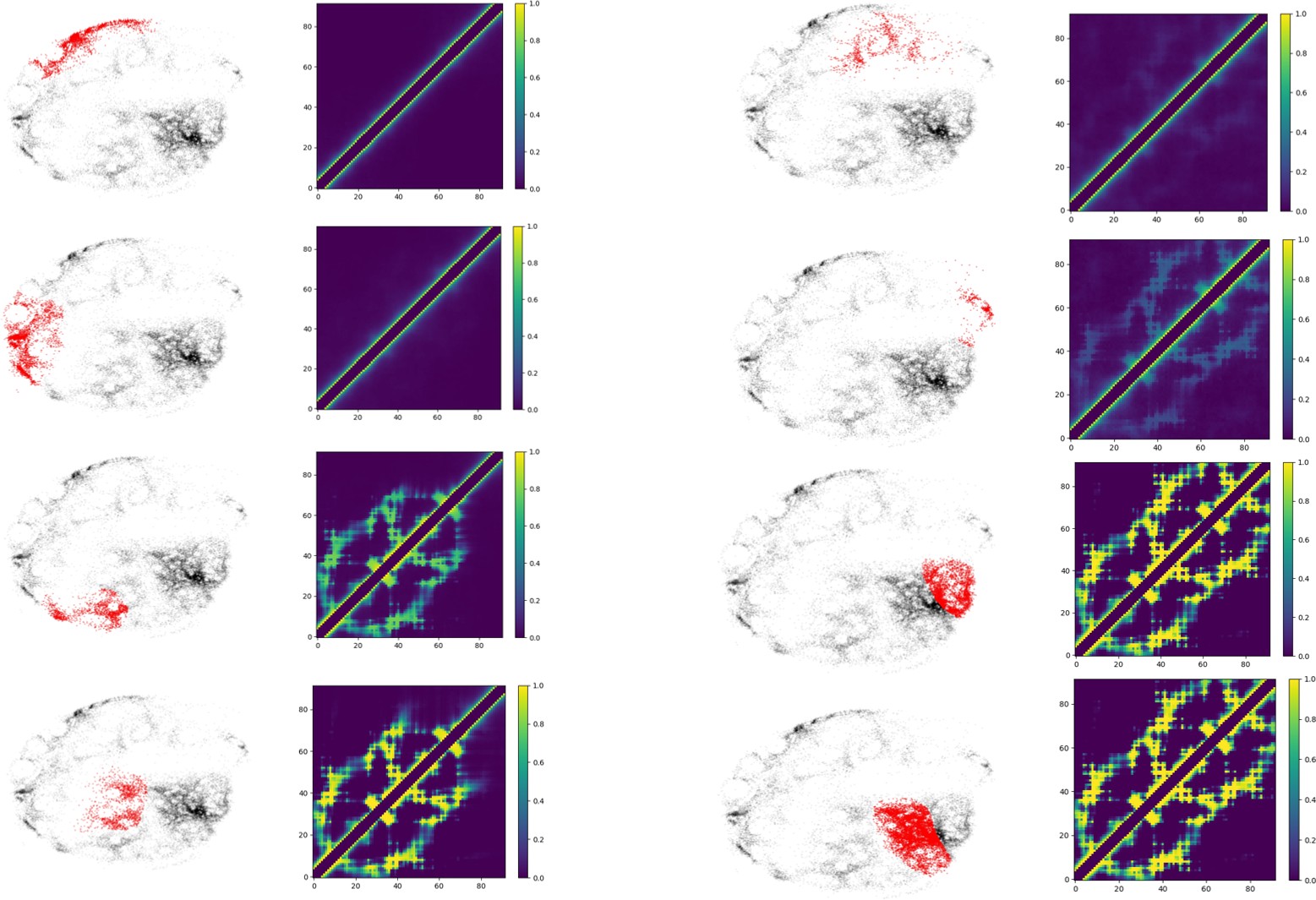


Figure S2: Mean contact maps of the 3ANK structures corresponding to the different regions of the ELViM projection (highlighted in red).

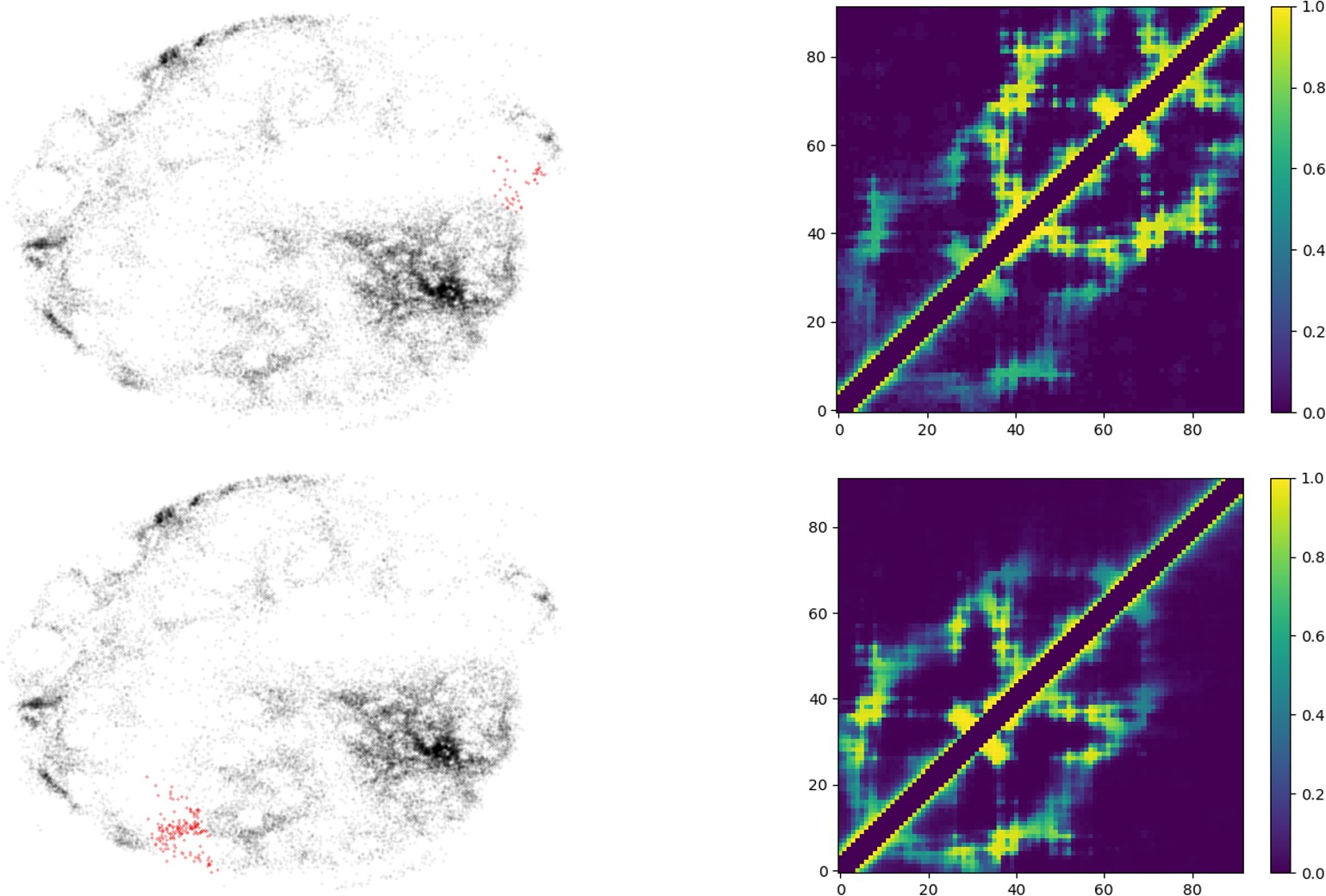


Figure S3: Mean contact maps of the 3ANK transition states with the same values of global *Qo*. The difference between these conformations combined with the fact that they have similar *Qo* values is the reason behind the apparent backtracking.

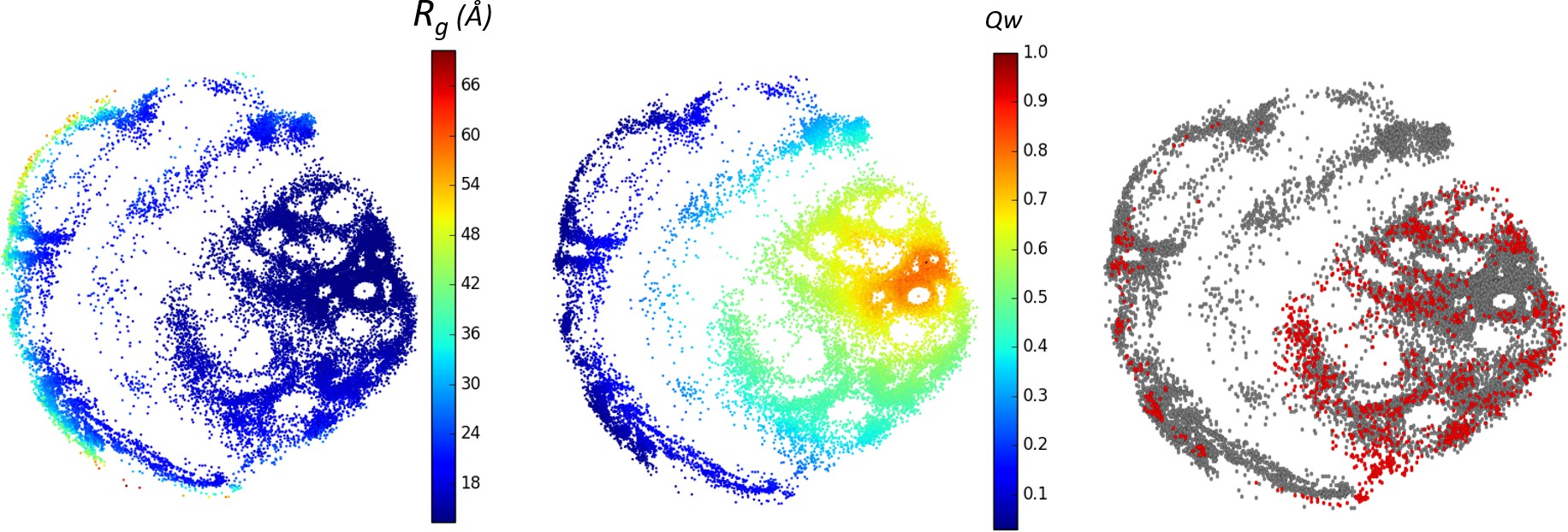


Figure S4: ELViM 2D projection of the conformational phase space of 4ANK as (A) a function of the radius of gyration and (b) a function of *Qw* coordinate. (c) Projection showing the conformations obtained with two different simulations: the unbiased conformations in red, and the biased conformations in grey.

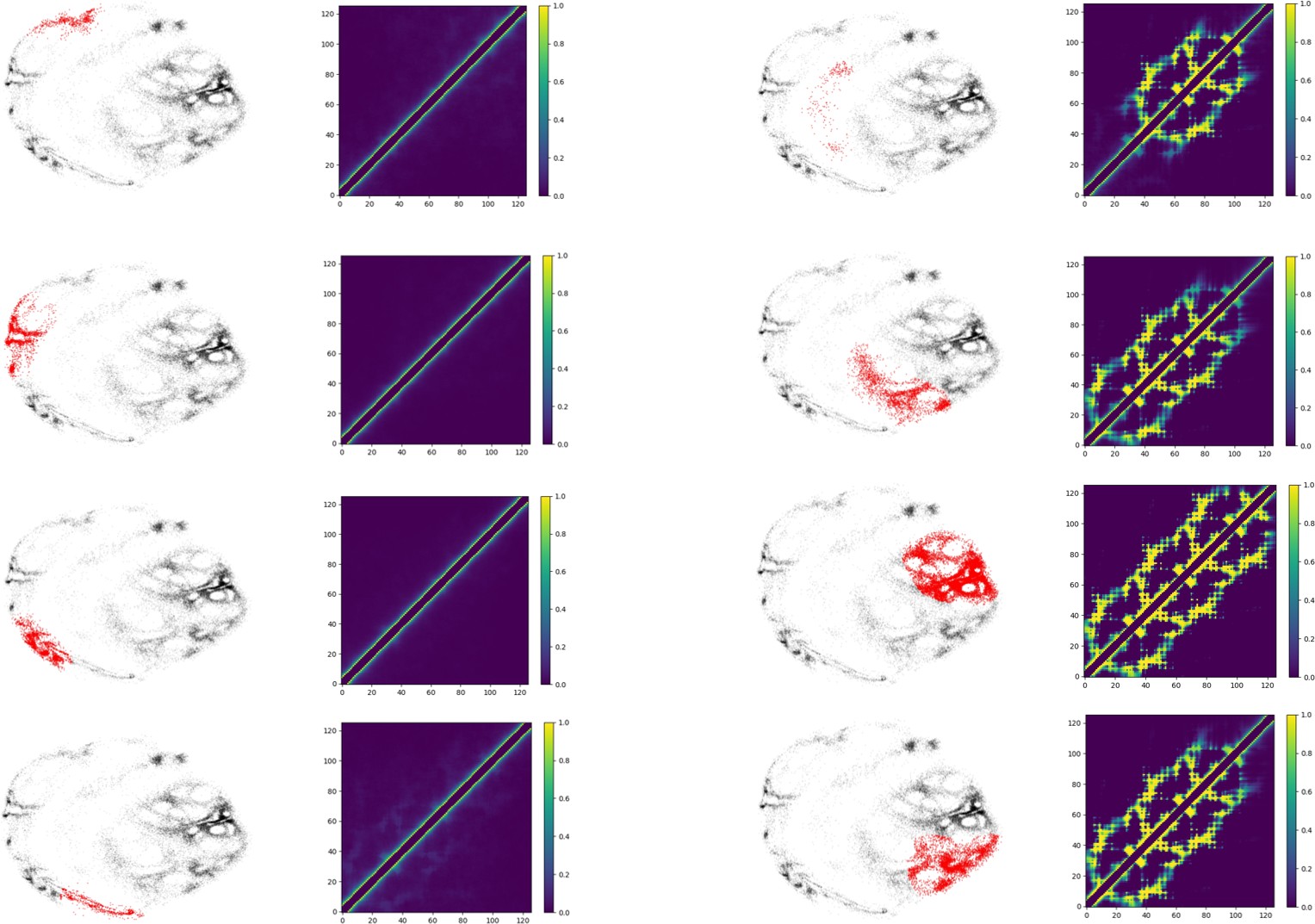


Figure S5: Mean contact maps of the 4ANK structures corresponding to the different regions of the ELViM projection (highlighted in red).

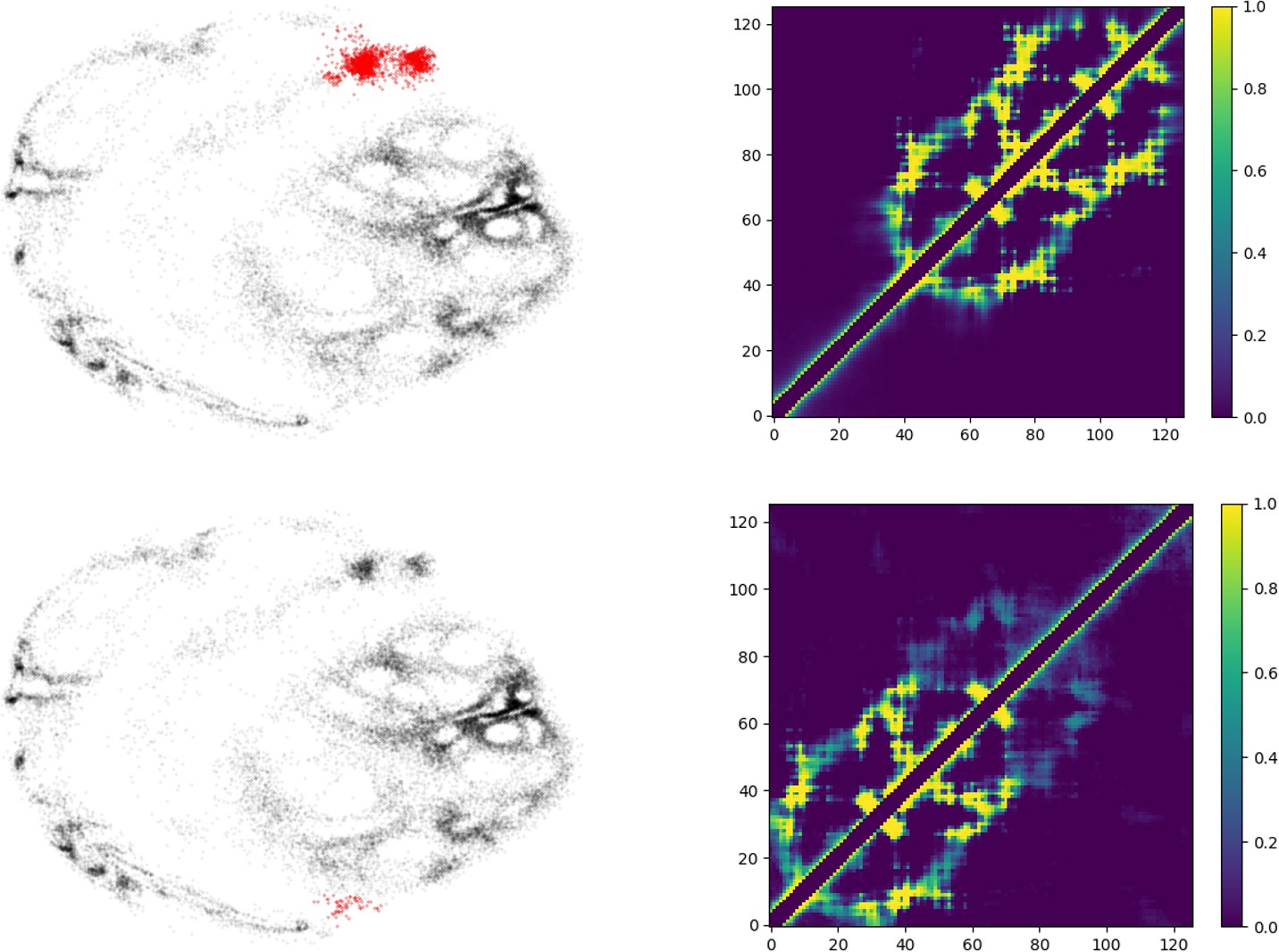


Figure S6: Mean contact maps of the 4ANK transition states with the same values of global *Qo*. The difference between these conformations combined with the fact that they have similar *Qo* values is the reason behind the apparent backtracking.

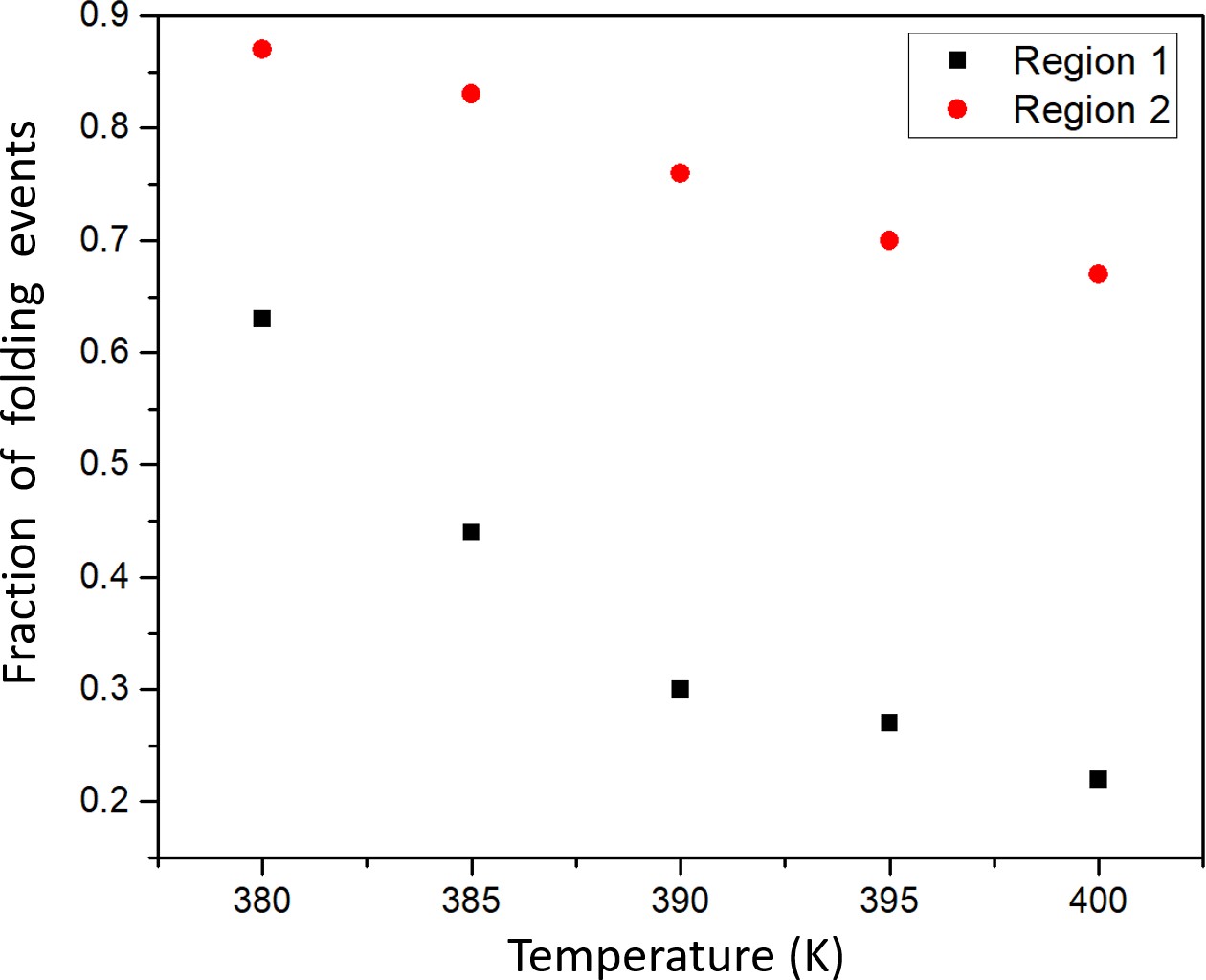


Figure S7: Fraction of folding events for region 1 and region 2 of the 4ANK for each different temperature.

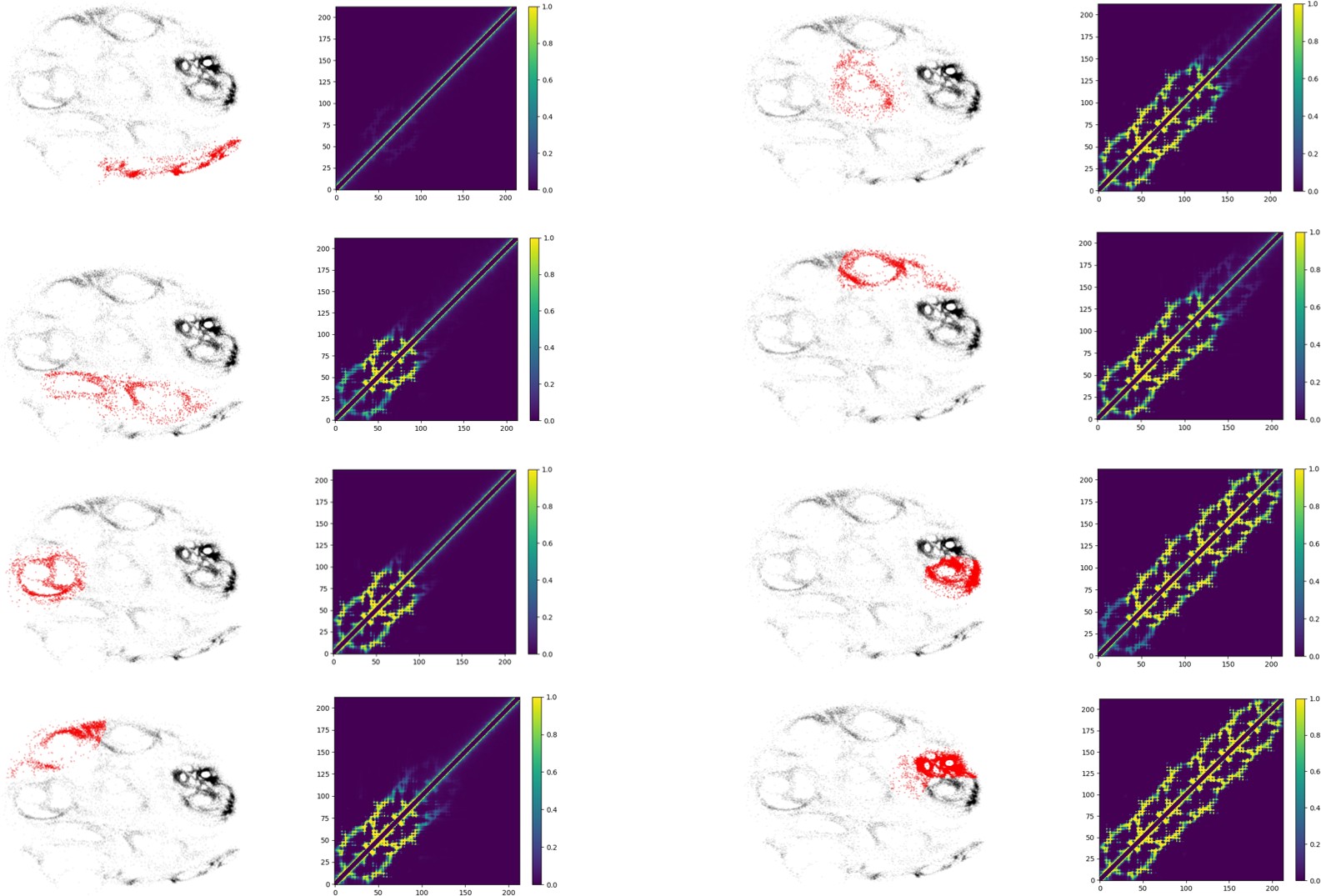


Figure S8: Mean contact maps of the 6ANK structures corresponding to the different regions of the ELViM projection (highlighted in red).

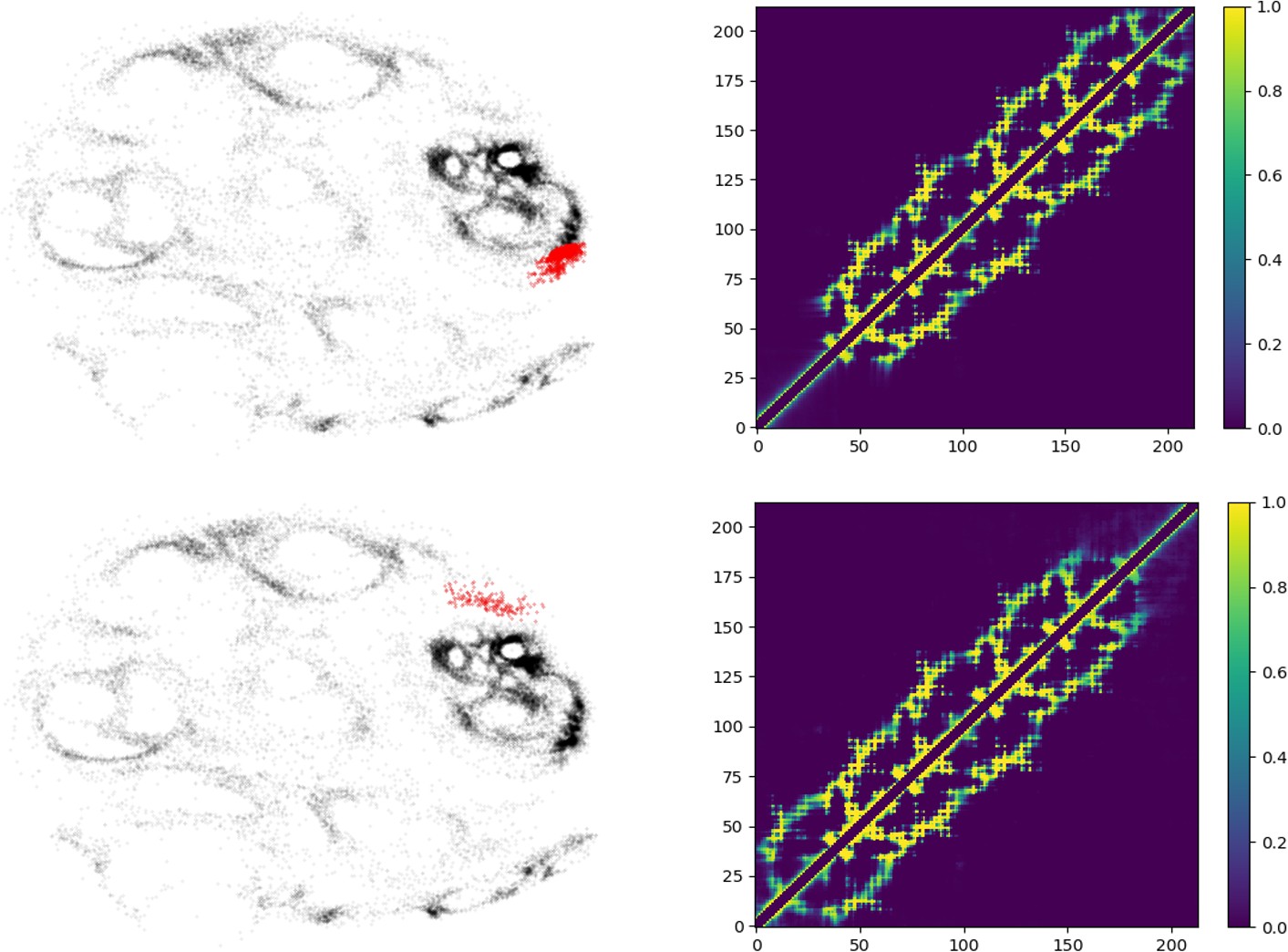


Figure S9: Mean contact maps of the 6ANK transition states with the same values of global *Qo*. The difference between these conformations combined with the fact that they have similar *Qo* values is the reason behind the apparent backtracking.

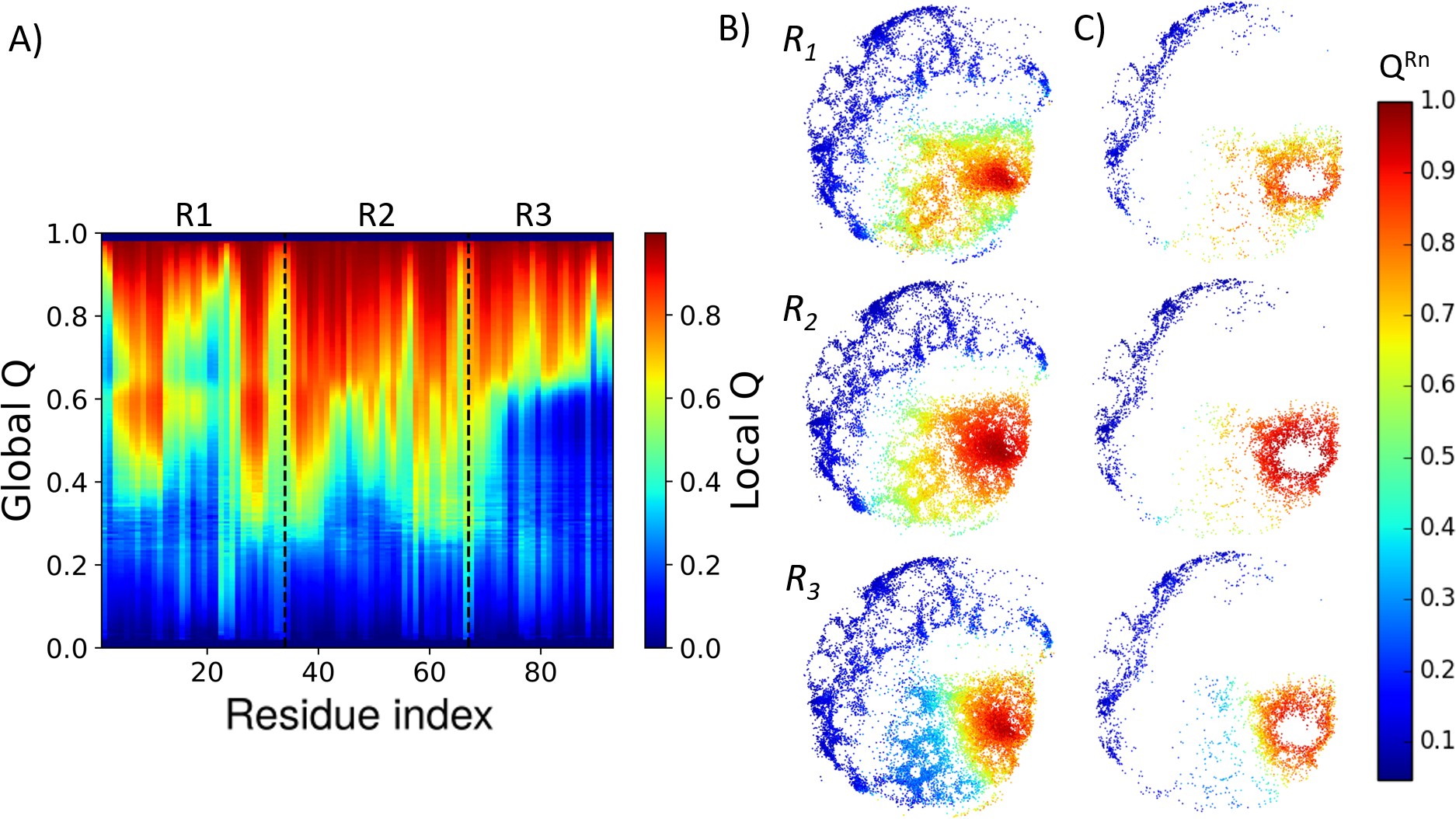


Figure S10: (a) Degree of folding of each residue as a function of *Qo*. The color indicates the average local *Qoi* for a specific residue *i* over the entire set of structures of a given global *Qo* for 3ANK. (b) 2-dimensional ELViM projections for 3ANK biased trajectories, as a function of *QoRn* for each repeat. (c) 2-dimensional ELViM projections for 3ANK unbiased trajectories, as a function of *QoRn* for each repeat

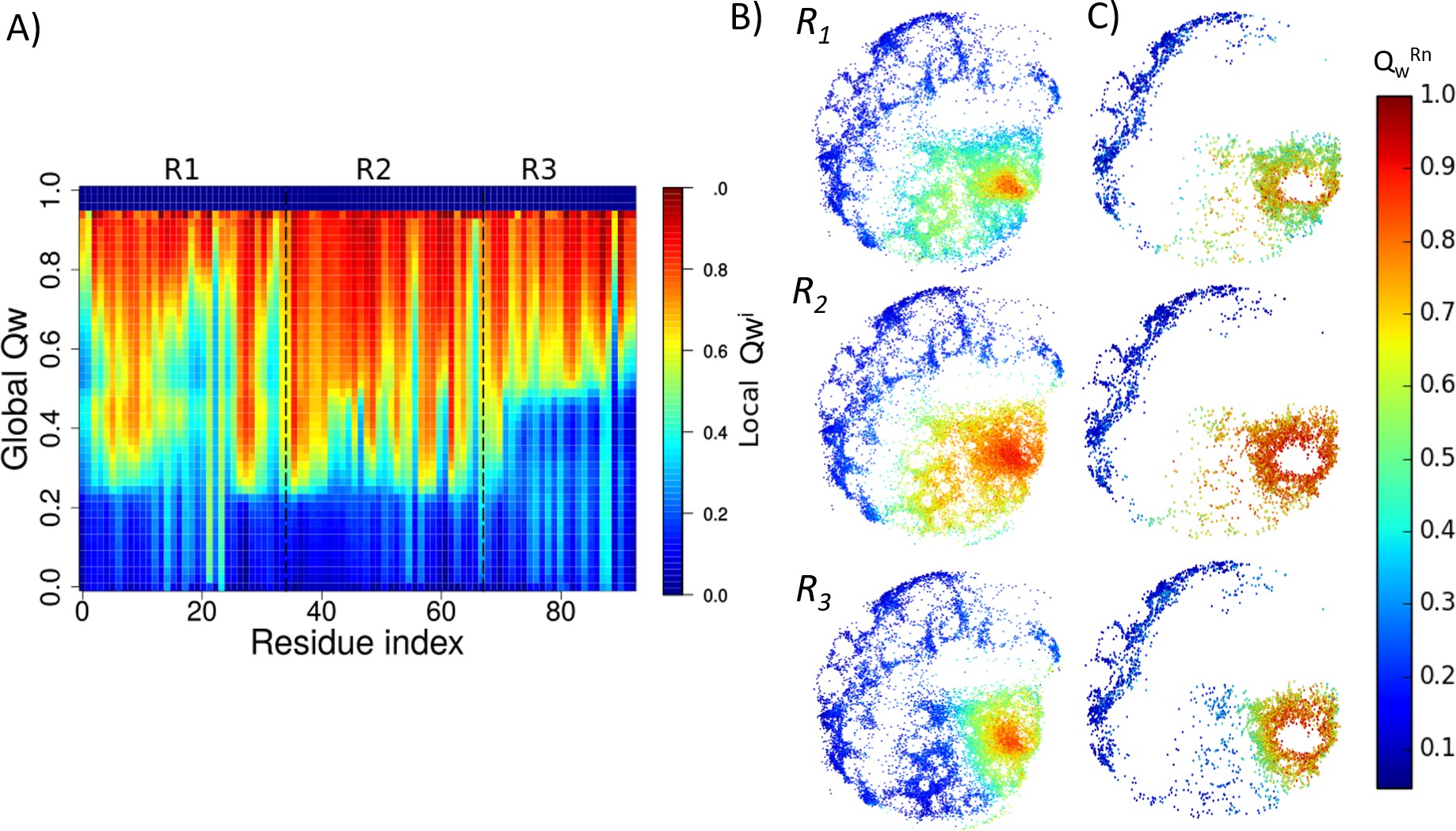


Figure S11: (a) Degree of folding of each residue as a function of *Qw*. The color indicates the average local *Qwi* for a specific residue *i* over the entire set of structures of a given global *Qw* for 3ANK. (b) 2-dimensional ELViM projections for 3ANK biased trajectories, as a function of *QwRn* for each repeat. (c) 2-dimensional ELViM projections for 3ANK unbiased trajectories, as a function of *QwRn* for each repeat.

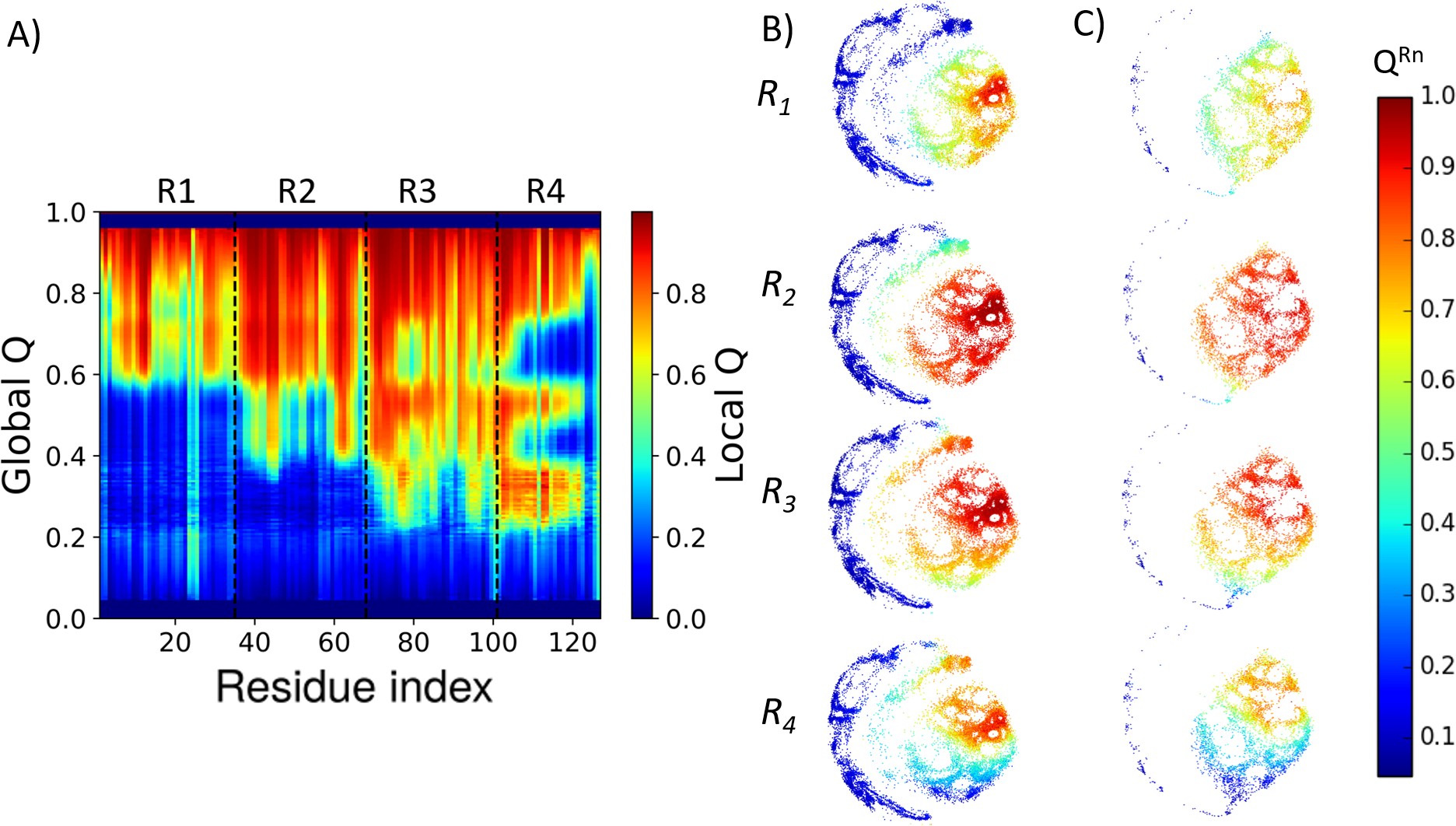


Figure S12: Analyses of the 4ANK repeats formation. (a) Degree of folding of each residue as a function of *Qo*. The color indicates the average local *Qoi* for a specific residue *i* over the entire set of structures of a given global *Qo* for 4ANK. (b) 2-dimensional ELViM projections for 4ANK biased trajectories, as a function of *QoRn* for each repeat. (c) 2-dimensional ELViM projections for 4ANK unbiased trajectories, as a function of *QoRn* for each repeat.

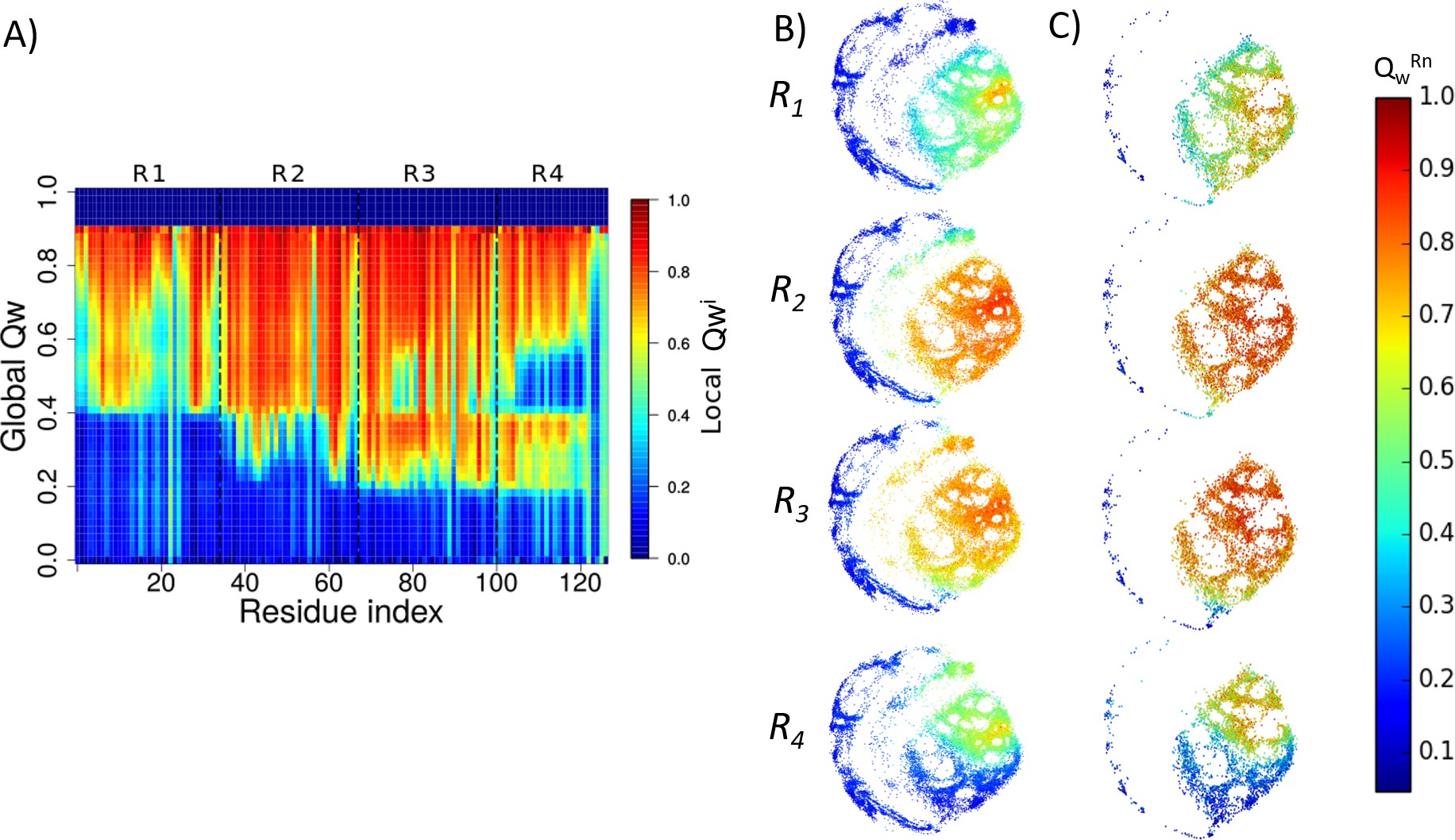


Figure S13: Analyses of the 4ANK repeats formation. (a) Degree of folding of each residue as a function of *Qw*. The color indicates the average local *Qwi* for a specific residue *i* over the entire set of structures of a given global *Qw* for 4ANK. (b) 2-dimensional ELViM projections for 4ANK biased trajectories, as a function of *QwRn* for each repeat. (c) 2- dimensional ELViM projections for 4ANK unbiased trajectories, as a function of *QwRn* for each repeat

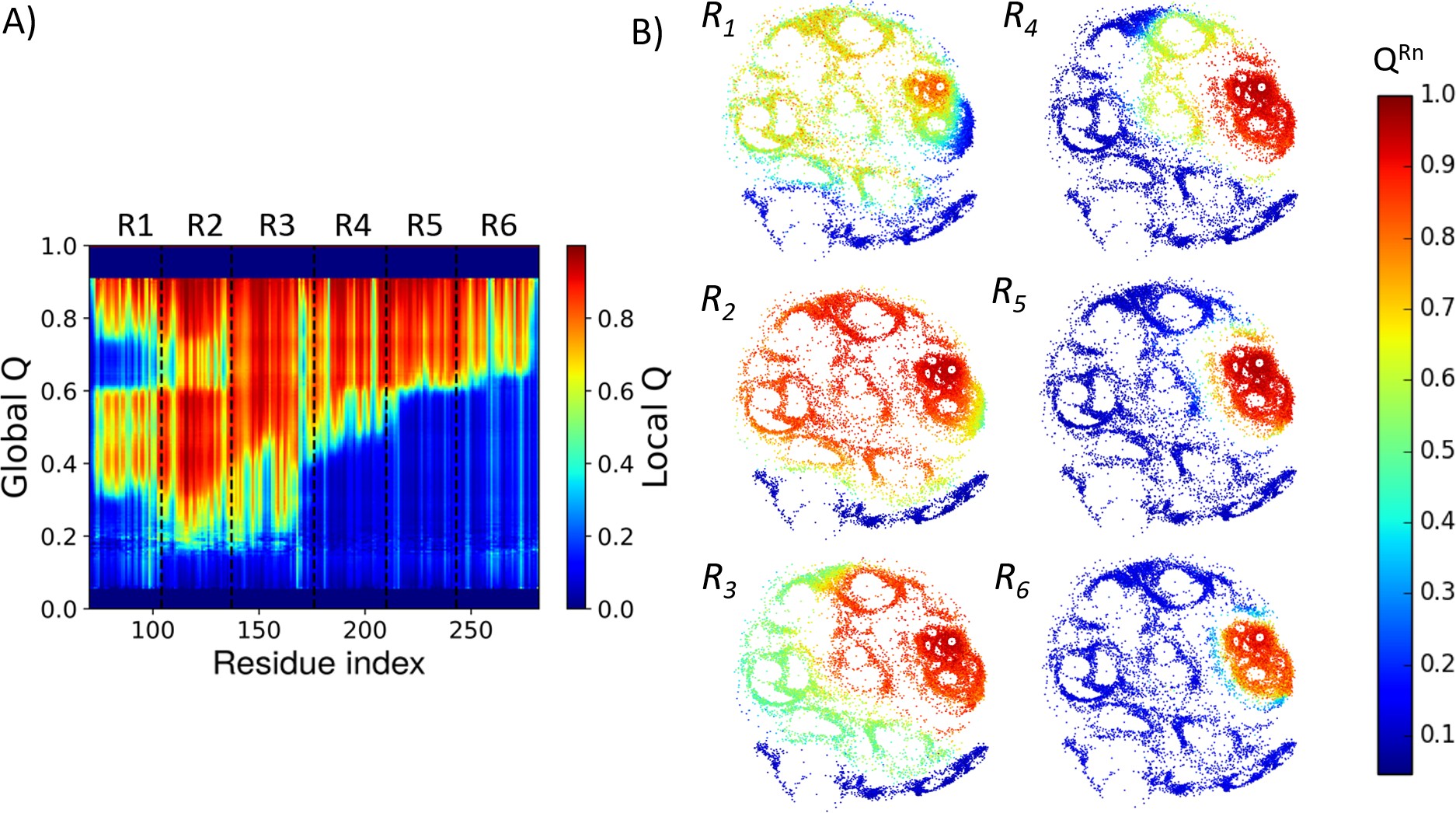


Figure S14: (a) Degree of folding of each residue as a function of *Qo*. The color indicates the average local *Qoi* for a specific residue *i* over the entire set of structures of a given global *Qo* for 6ANK. (b) 2-dimensional ELViM projections of 6ANK biased trajectories, as a function of *QoRn* for each repeat.

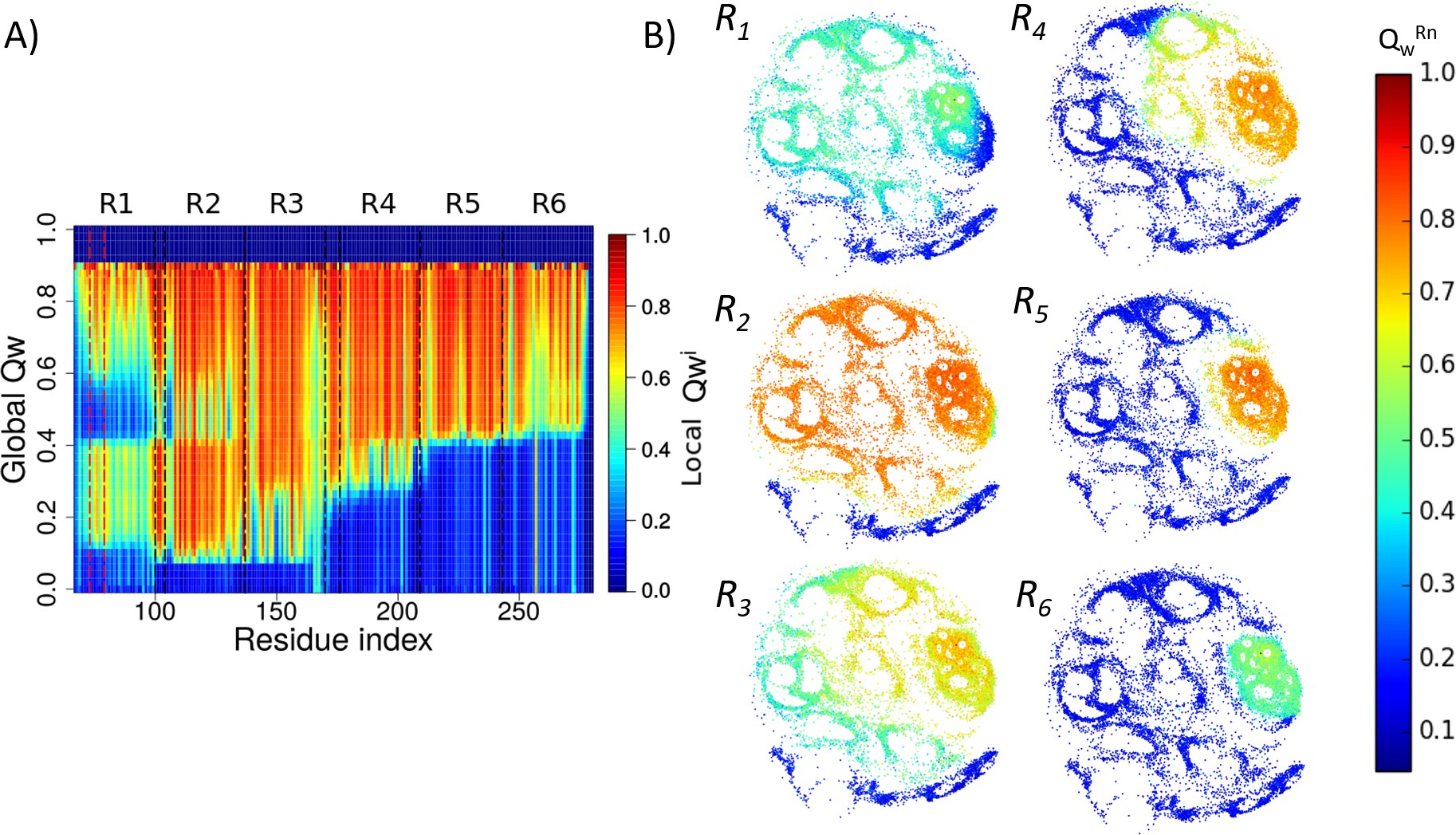


Figure S15: (a) Degree of folding of each residue as a function of *Qw*. The color indicates the average local *Qwi* for a specific residue *i* over the entire set of structures of a given global *Qw* for 6ANK. (b) 2-dimensional ELViM projections of 6ANK biased trajectories, as a function of *QwRn* for each repeat.