

Essential Dynamics of Ubiquitin in Water and in a Natural Deep Eutectic Solvent

SUPPORTING INFORMATION

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S1. Principal Component Analysis of Ubiquitin at 298 K

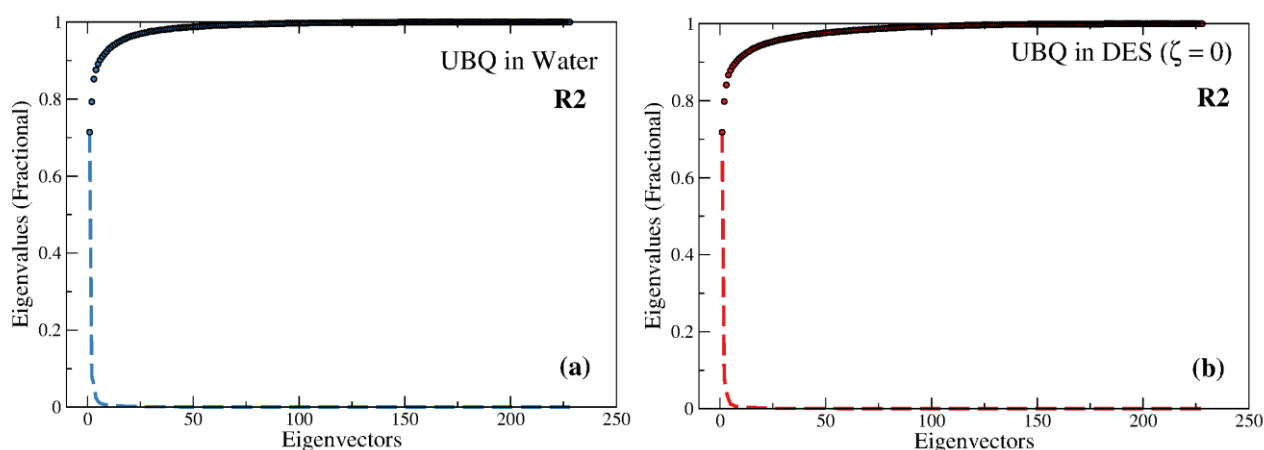


Figure S1 - Cartesian coordinates covariance (cov) matrix 228 eigenvalues, in decreasing order of magnitude at 298 K and 0.1MPa, for UBQ in **(a)** water, and **(b)** (B:G:W) (1:2: ζ ; $\zeta = 0$). The 228 $\times$ 228 cov matrix was computed for the Cartesian position coordinates of UBQ's C $_{\alpha}$ atoms (76 C $_{\alpha}$ atoms). The circles represent the respective cumulative sum of the eigenvalues.

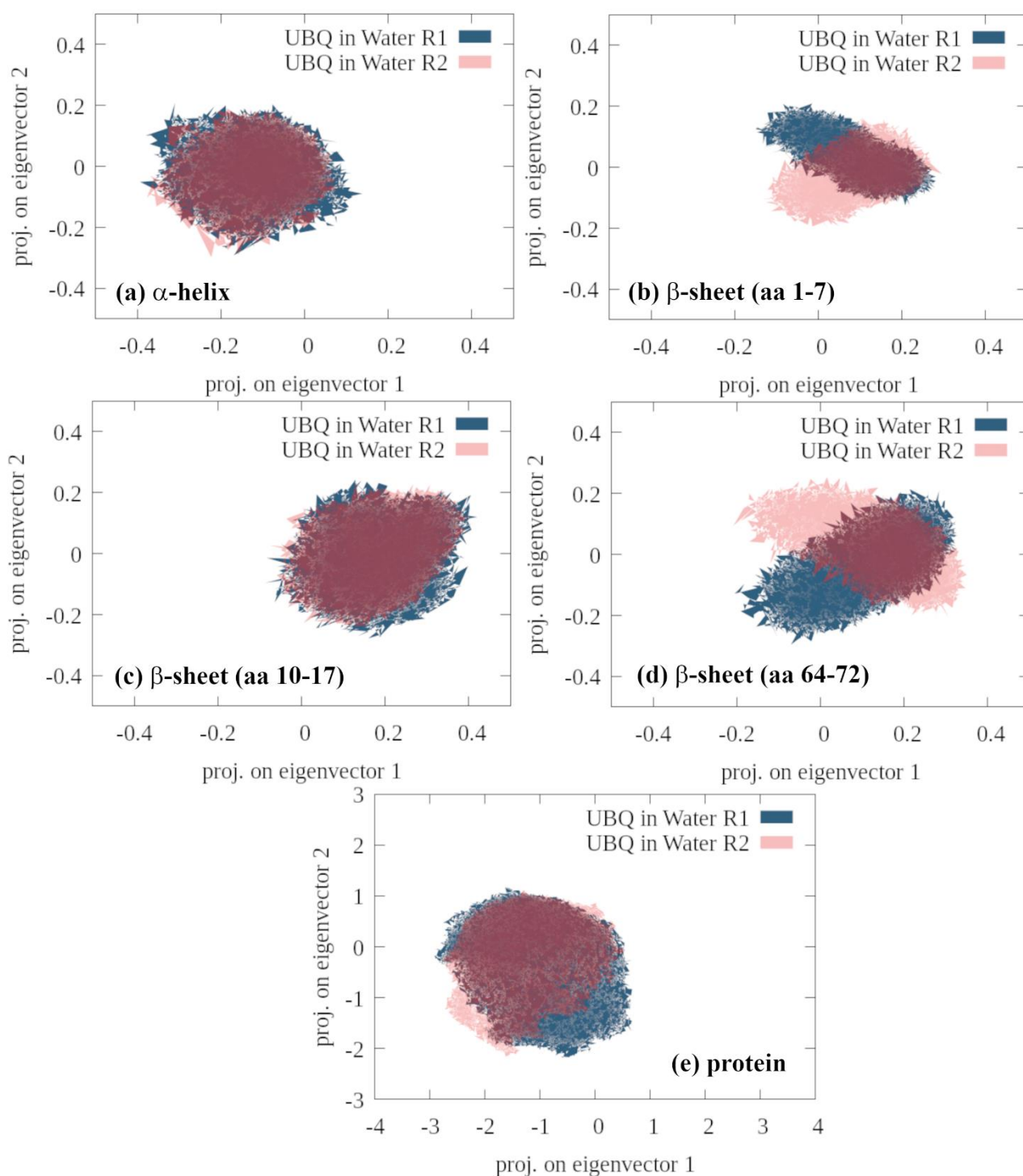


Figure S2 – PCA atomic displacement projections in the plane formed by the first two eigenvectors at 298 K and 0.1 MPa in neat water for two MD replicates (R1 and R2). The projections for the C_α of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used.

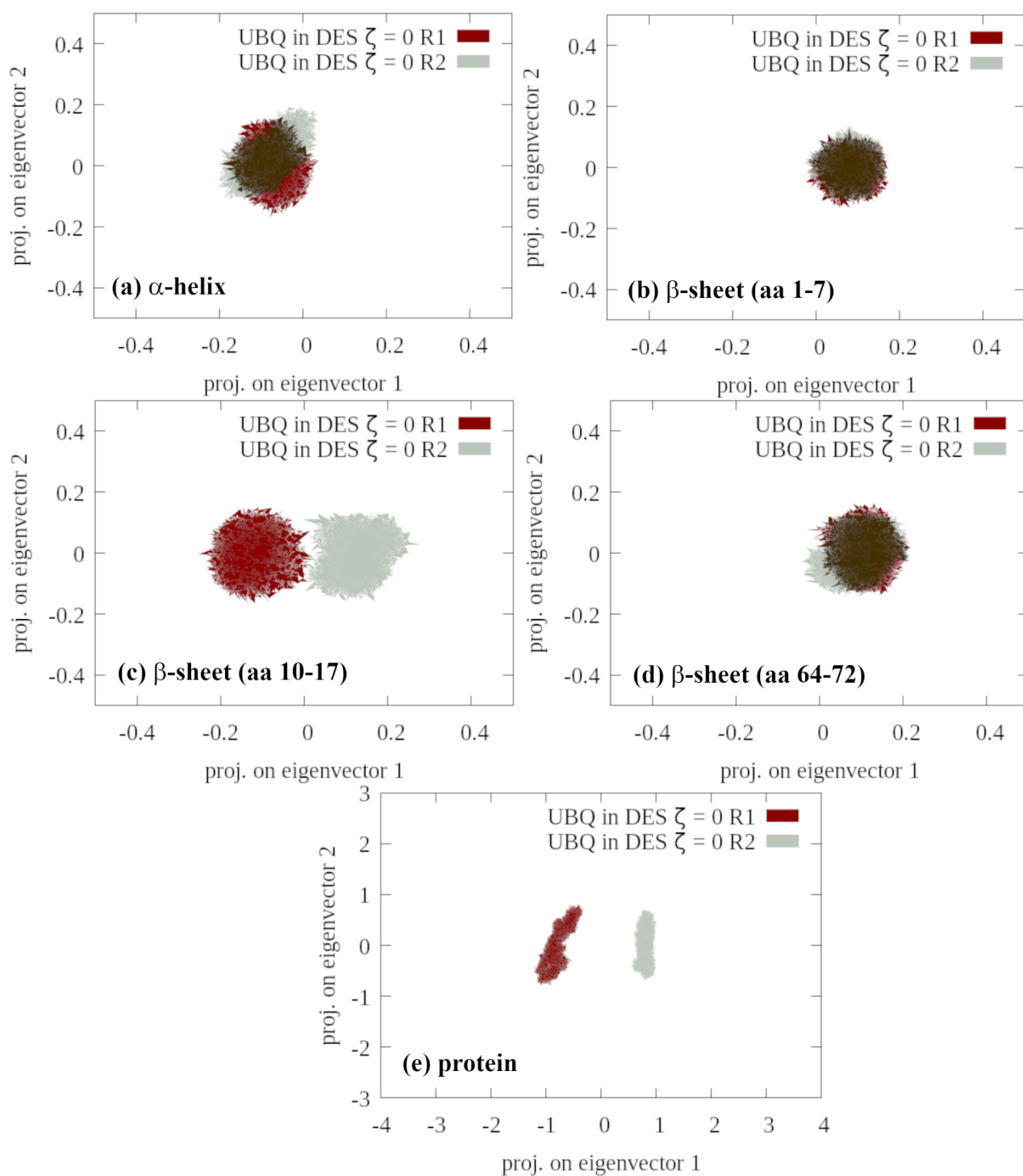


Figure S3 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in anhydrous DES (B:G:W) (1:2:ζ=0) at 298 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C_{α} of the **(a)** α-helix, **(b)** β-sheet (aa 1-7), **(c)** β-sheet (aa 10-17), **(d)** β-sheet (aa 64-72), and **(e)** protein are displayed. Transparency is used.

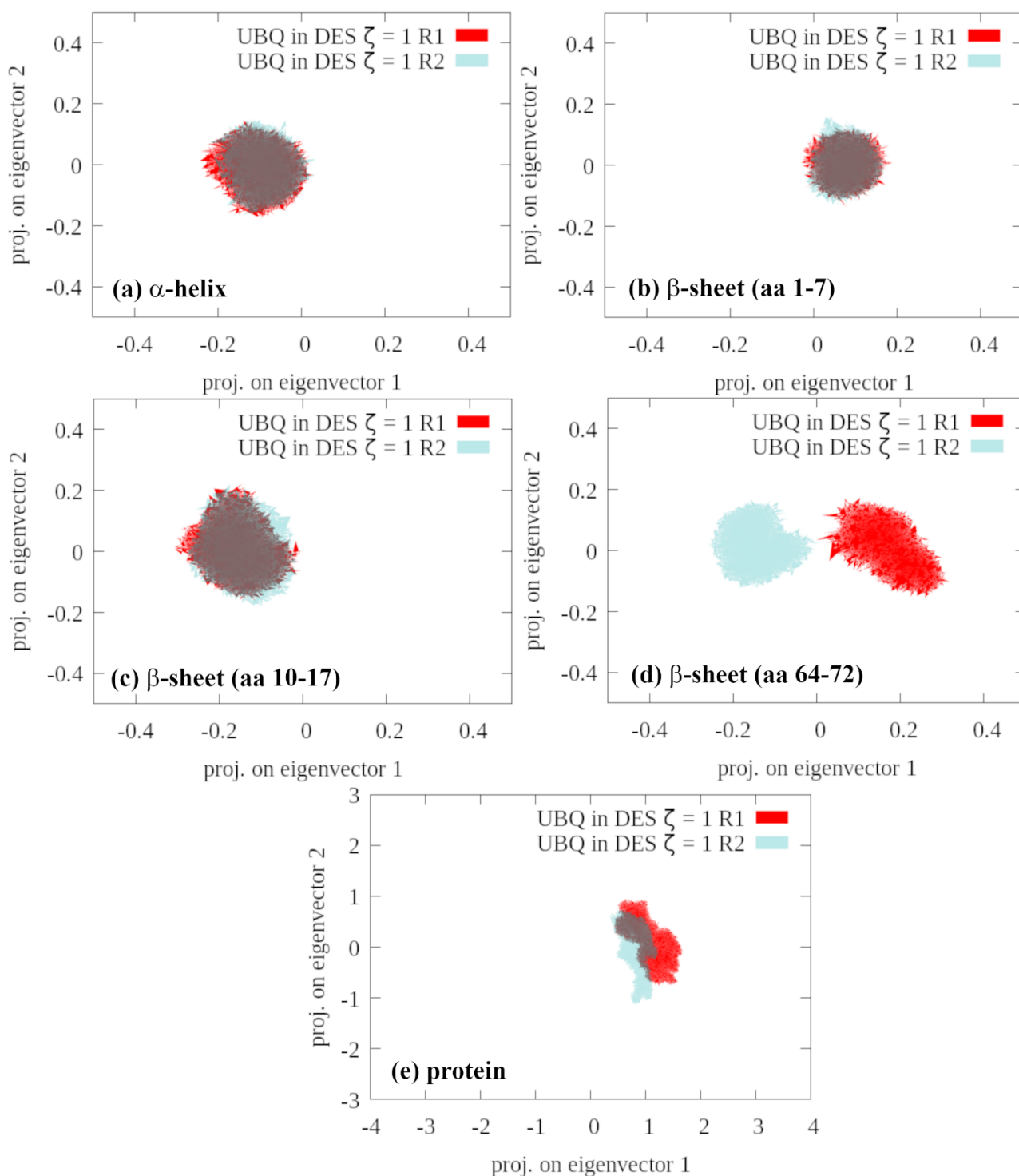


Figure S4 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in aqueous DES (B:G:W) (1:2:ζ=1) at 298 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C_{α} of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used.

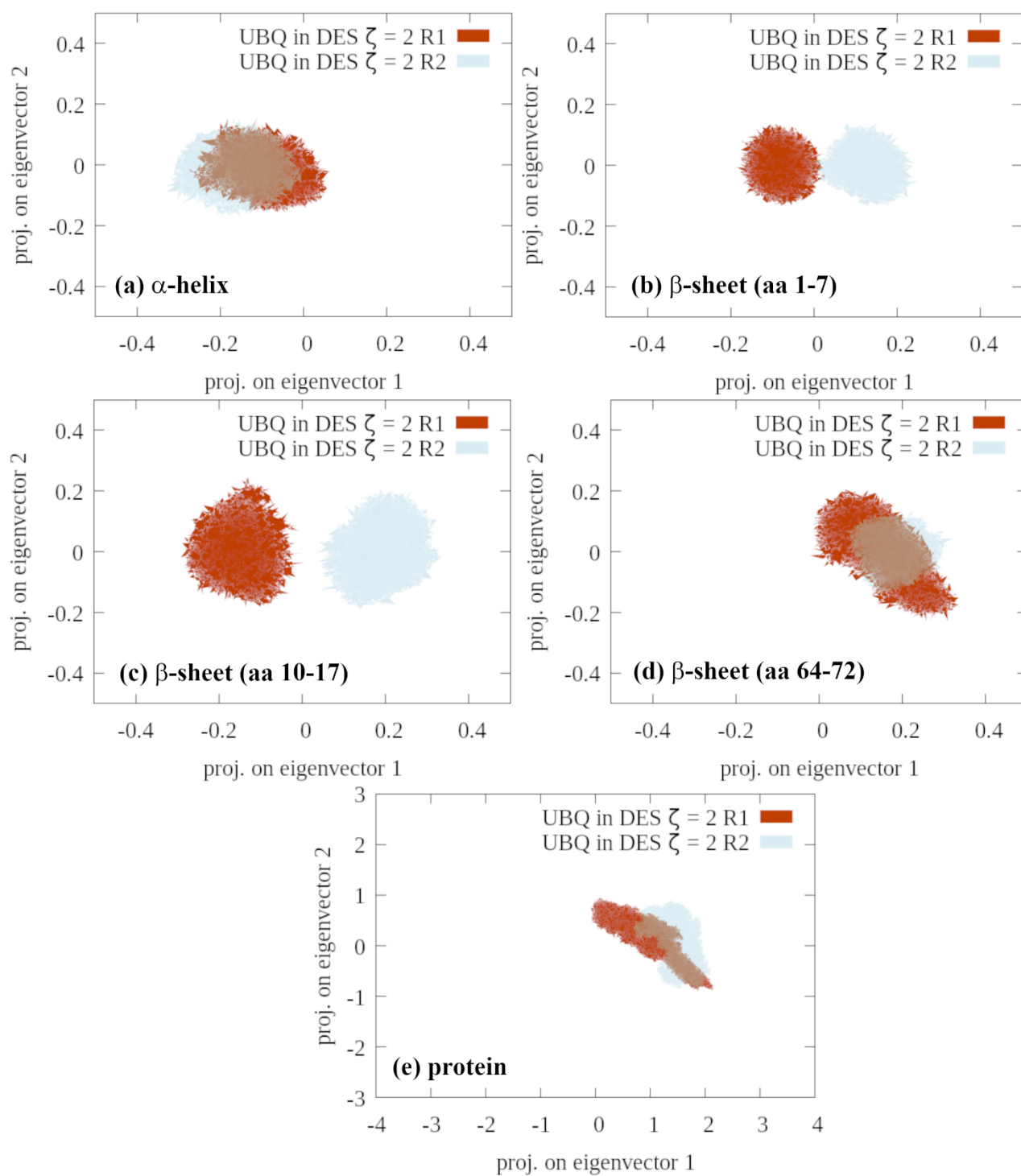


Figure S5 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in aqueous DES (B:G:W) (1:2:ζ=2) at 298 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C_{α} of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used.

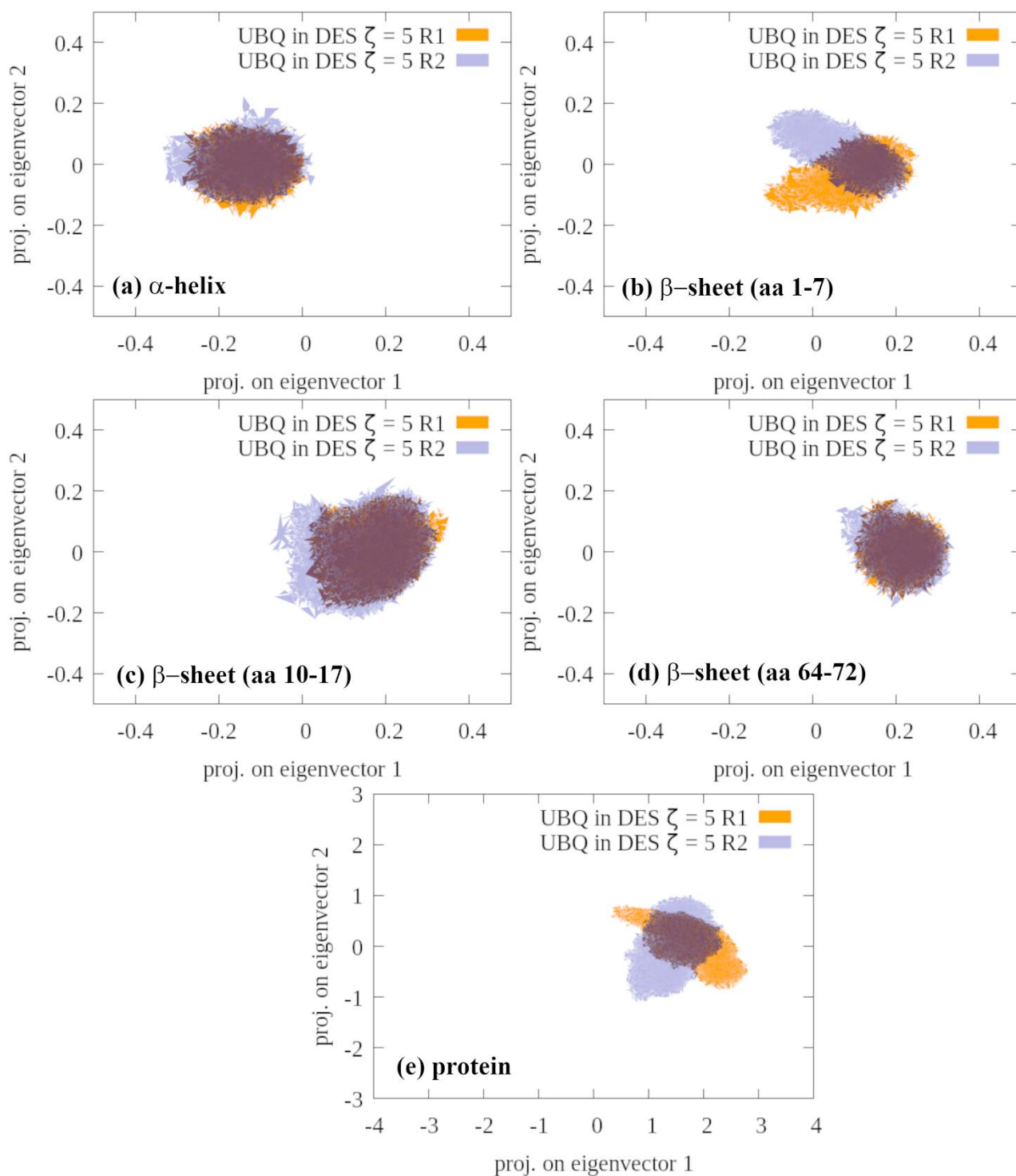


Figure S6 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in aqueous DES (B:G:W) (1:2:ζ=5) at 298 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C_α of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used.

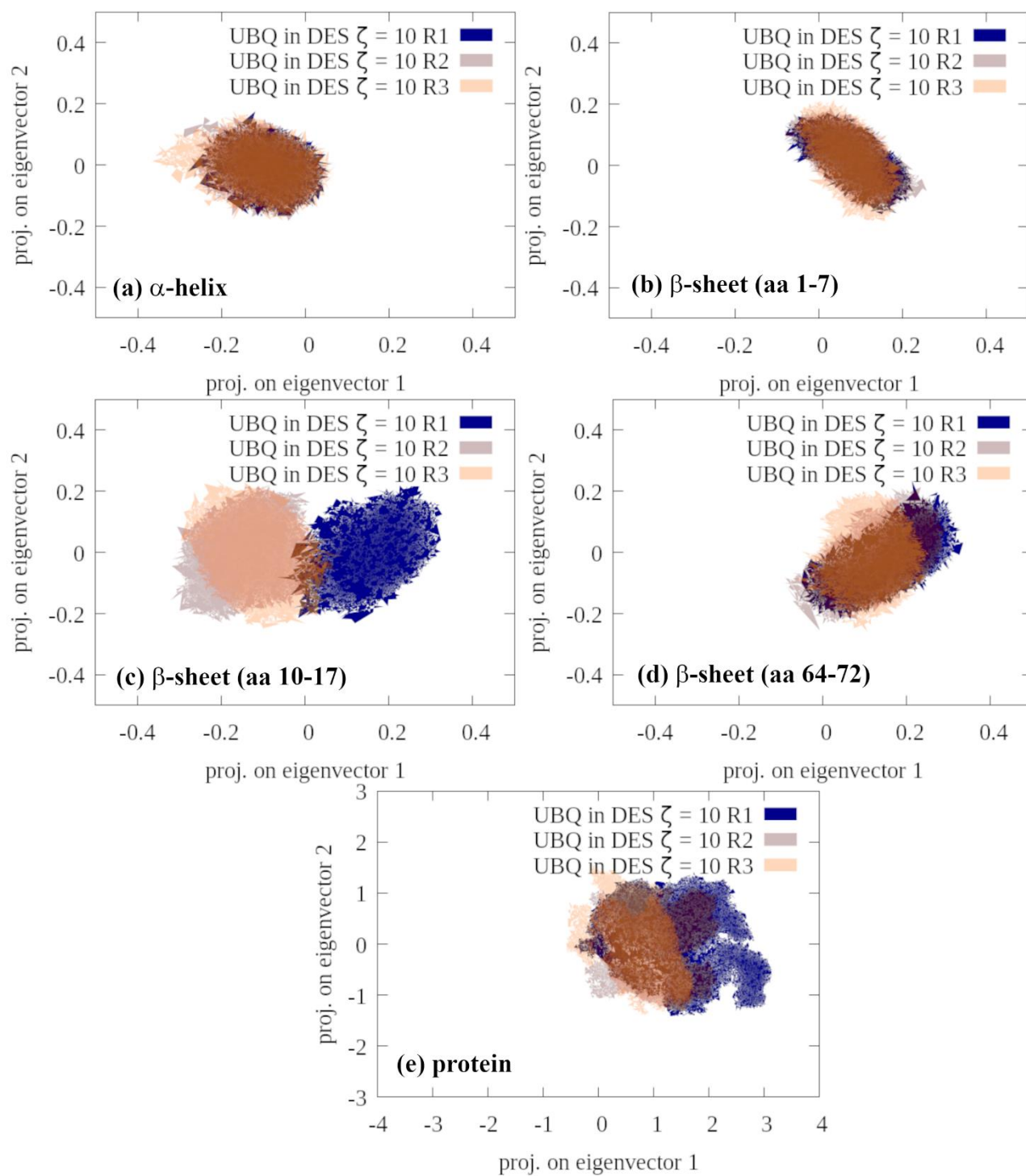


Figure S7 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in aqueous DES (B:G:W) (1:2: $\zeta=10$) at 298 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C_α of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used.

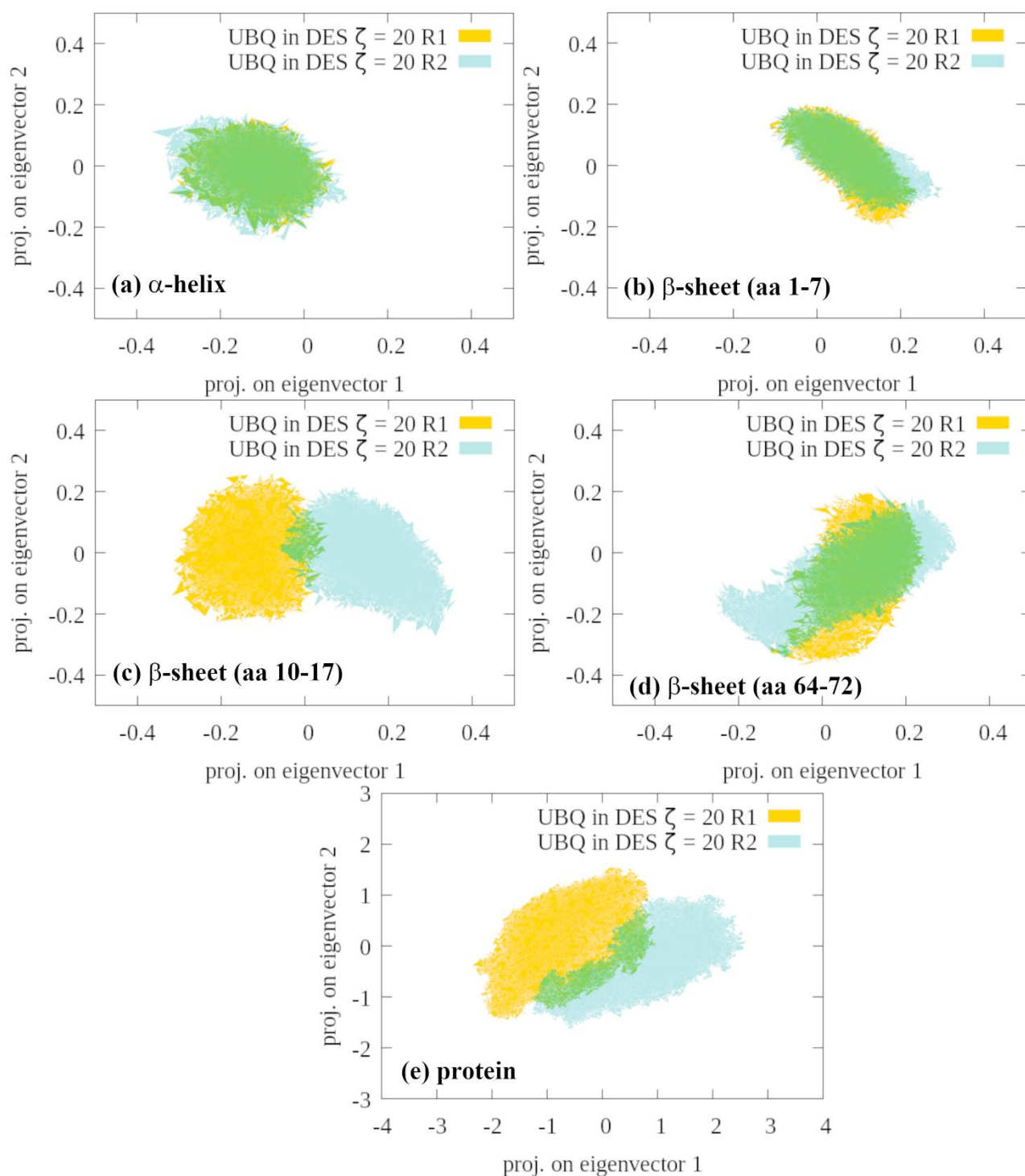


Figure S8 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in aqueous DES (B:G:W) (1:2:ζ=20) at 298 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C_α of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used.

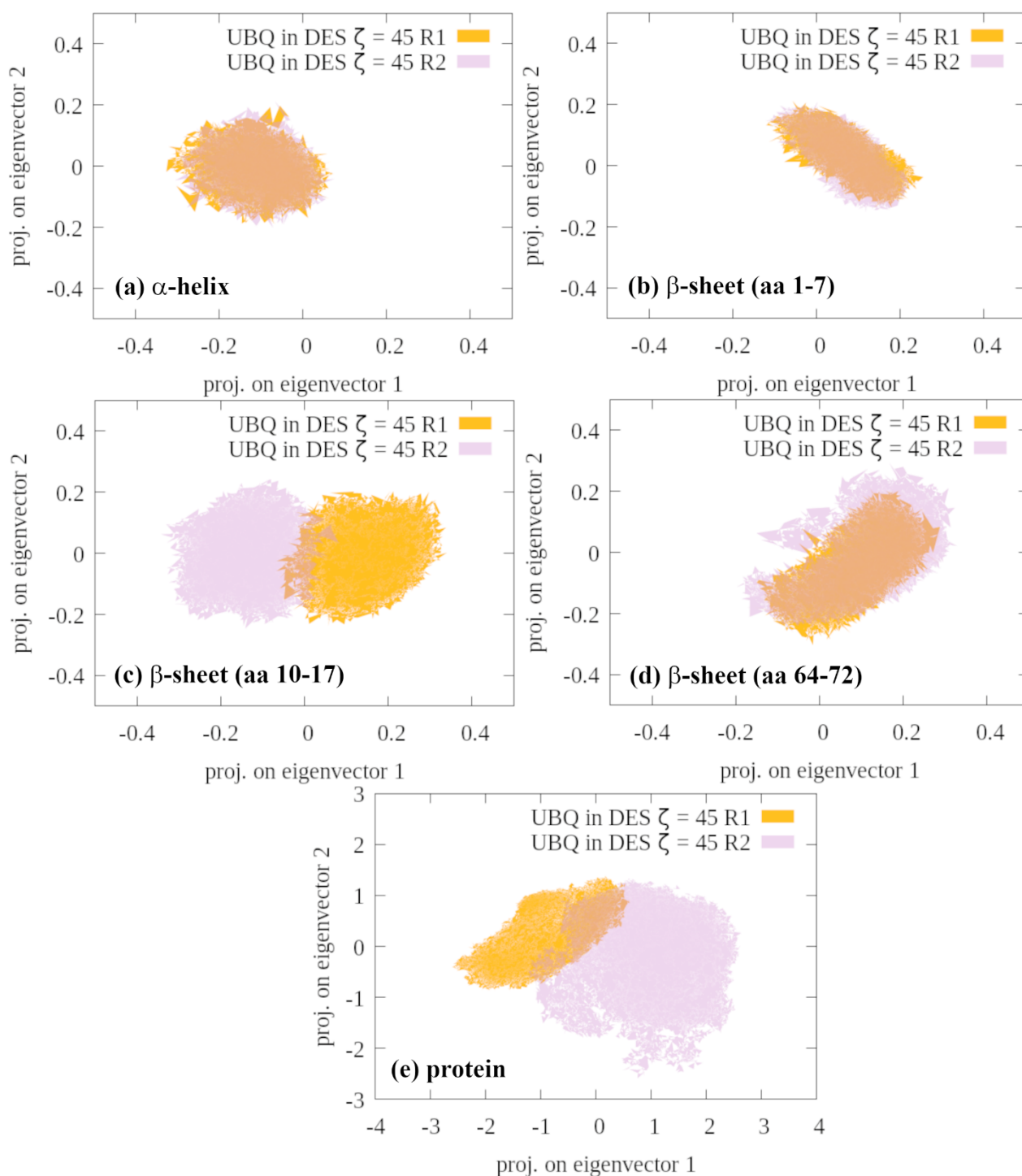


Figure S9 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in aqueous DES (B:G:W) (1:2:ζ=45) at 298 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C_α of the (a) α-helix, (b) β-sheet (aa 1-7), (c) β-sheet (aa 10-17), (d) β-sheet (aa 64-72), and (e) protein are displayed. Transparency is used.

S2. Principal Component Analysis of Ubiquitin at 425 K

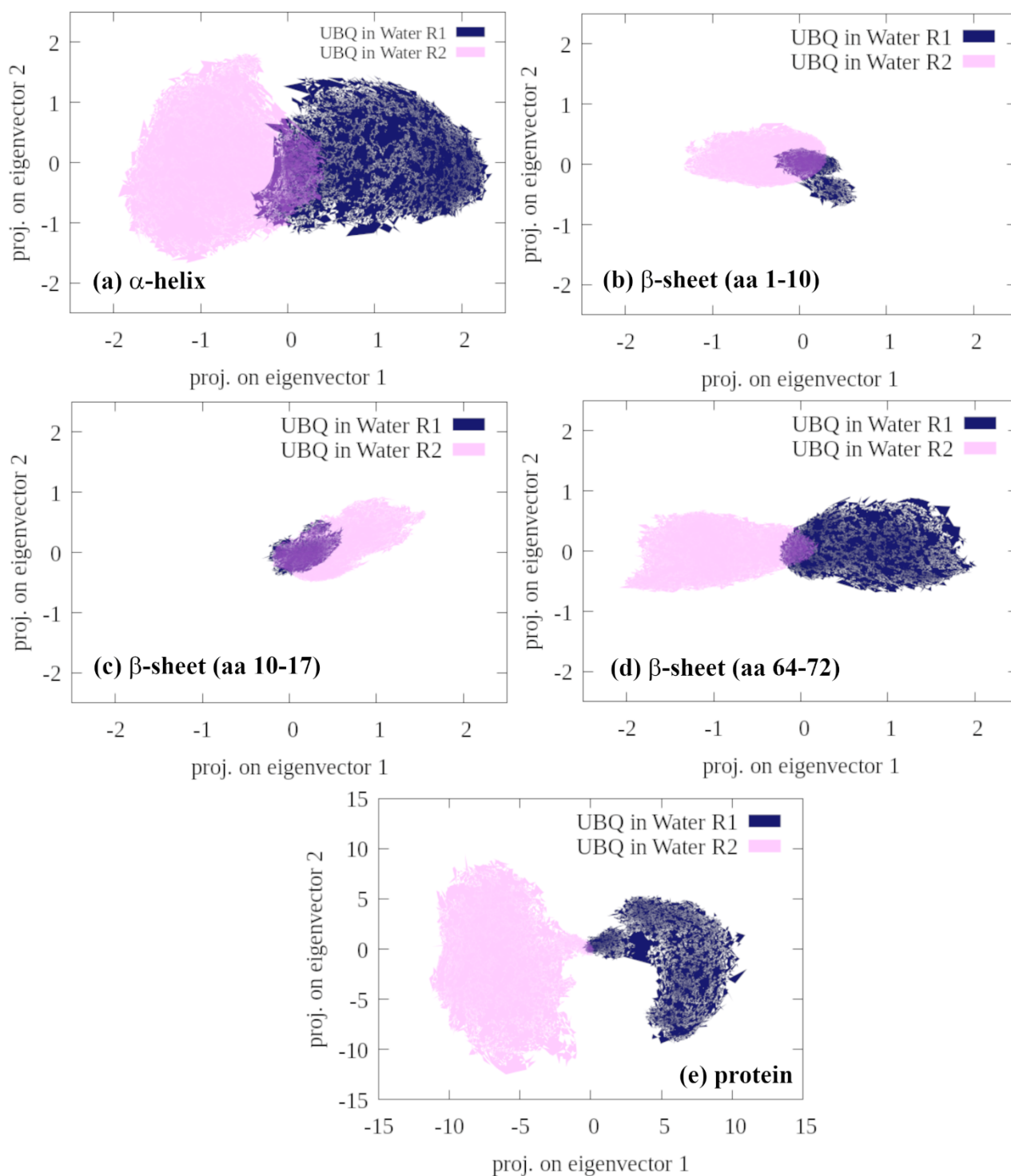


Figure S10 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in water at 425 K and 0.5 MPa for two MD replicates (R1 and R2). The projections for the C_α of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used. Please note the different scales used relative to Figs S2-S9.

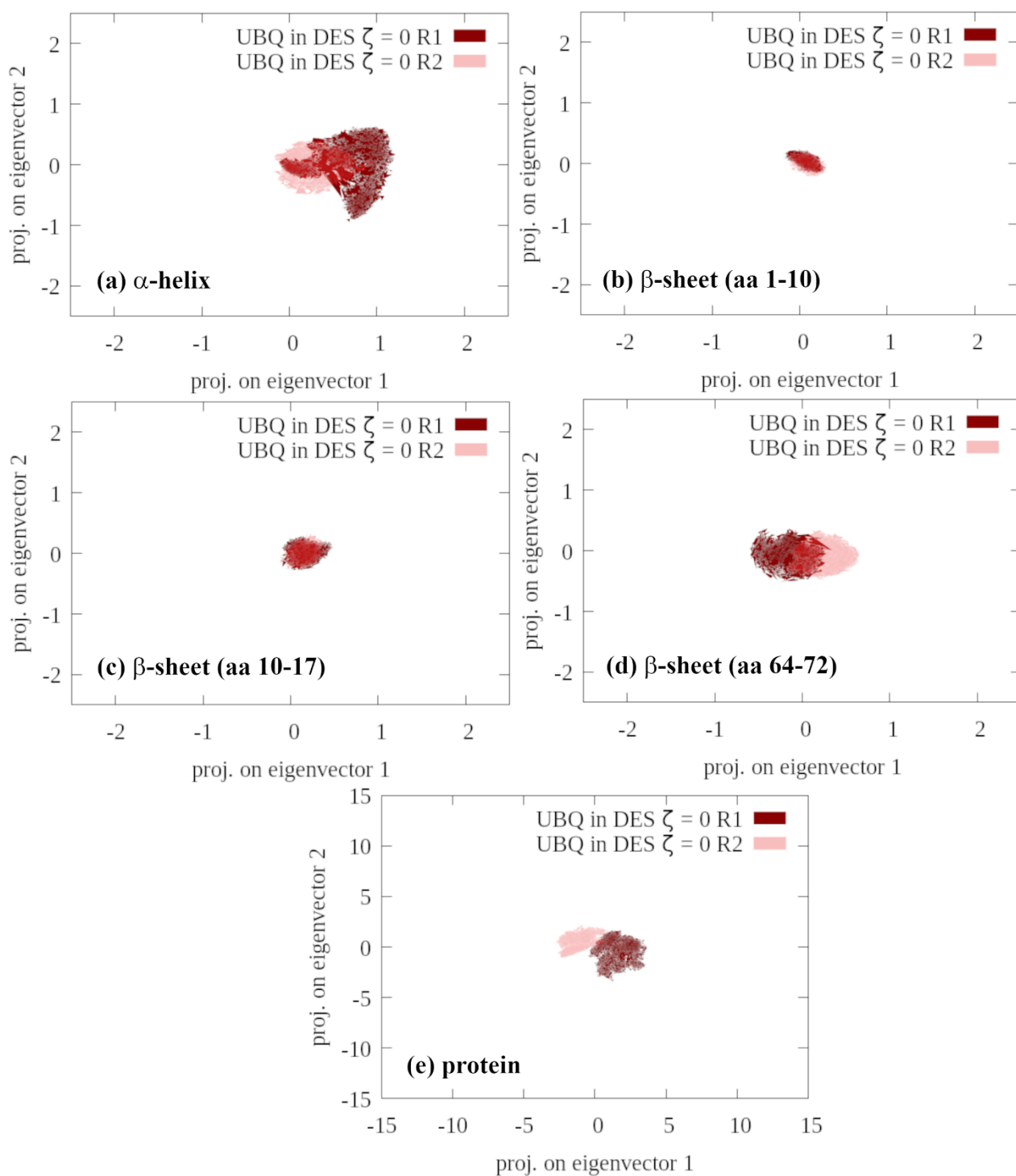


Figure S11 – PCA atomic displacement projections in the plane formed by the first two eigenvectors in anhydrous DES (B:G:W) (1:2: $\zeta=0$) at 425 K and 0.1 MPa for two MD replicates (R1 and R2). The projections for the C $_{\alpha}$ of the (a) α -helix, (b) β -sheet (aa 1-7), (c) β -sheet (aa 10-17), (d) β -sheet (aa 64-72), and (e) protein are displayed. Transparency is used. The same scales as in Fig. S10 are used.

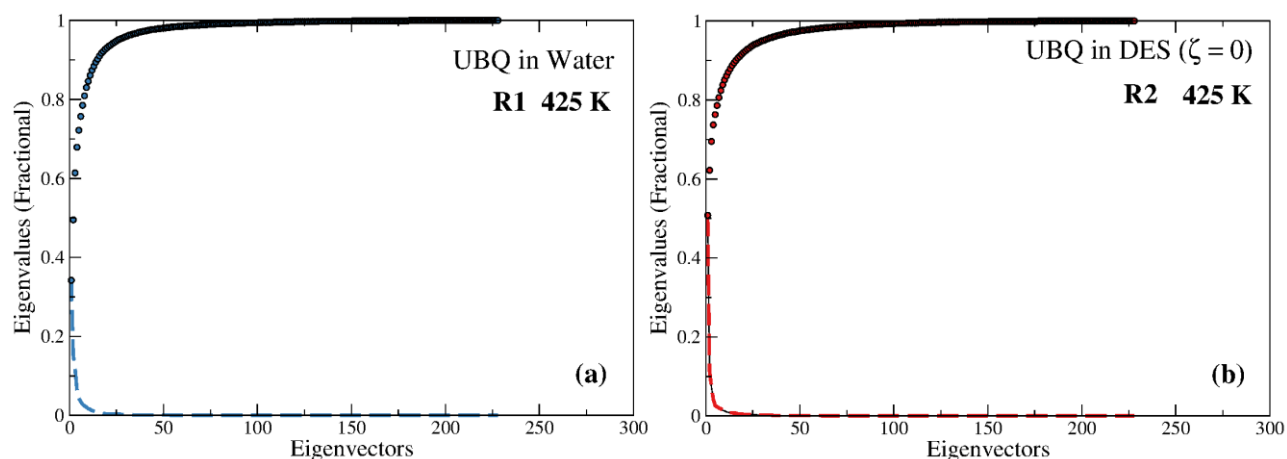


Figure S12 - Cartesian coordinates covariance (cov) matrix 228 eigenvalues, in decreasing order of magnitude at 425 K and 0.5MPa (water) and 0.1 MPa (DES), for UBQ in **(a)** water, and **(b)** (B:G:W) (1:2: ζ ; $\zeta = 0$). The 228 $\times$ 228 cov matrix was computed for the Cartesian position coordinates of UBQ's C_{α} atoms (76 C_{α} atoms). The circles represent the respective cumulative sum of the eigenvalues. An even larger difference is obtained between the other replicates leading to the average values reported in the manuscript.