

Supplementary Material for: Computing the Structural Dynamics of RVFV L Protein Domain in Aqueous Glycerol Solutions

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Summary of Simulations: Glycerol proportion (x_1) and water proportion (x_2).

| $x_1 : x_2$ | # atoms | Time (ns) | box size/side (Å) |
|-------------|---------|-----------------|-------------------|
| 100:00 | 43849 | 100×7 | 71.421 |
| 90:10 | 44230 | 100×5 | 71.527 |
| 80:20 | 44611 | 100×9 | 71.580 |
| 70:30 | 44992 | 100×5 | 71.961 |
| 60:40 | 45373 | 100×5 | 72.502 |
| 50:50 | 45754 | 100×10 | 73.061 |
| 40:60 | 46135 | 100×5 | 73.788 |
| 30:70 | 46516 | 100×4 | 74.225 |
| 20:80 | 46897 | 100×8 | 74.845 |
| 10:90 | 47278 | 100×7 | 75.470 |

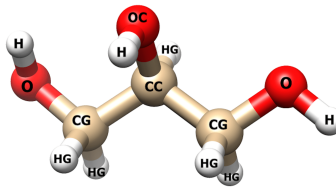
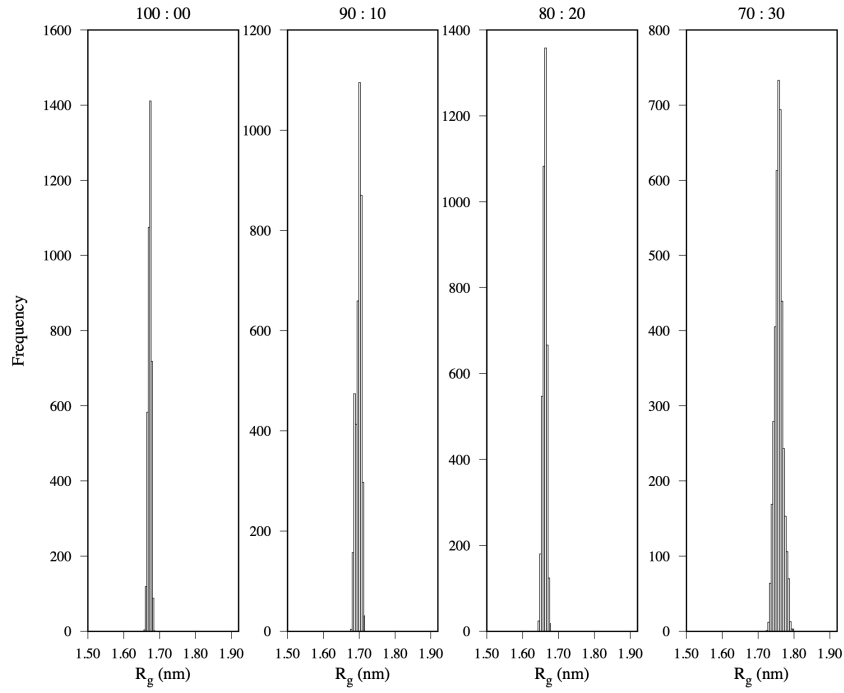


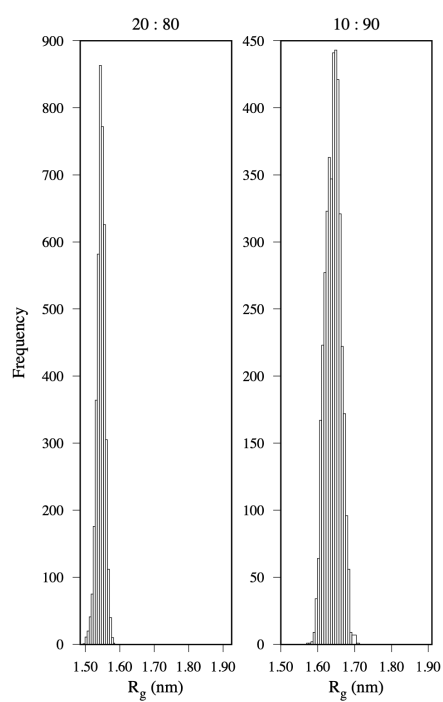
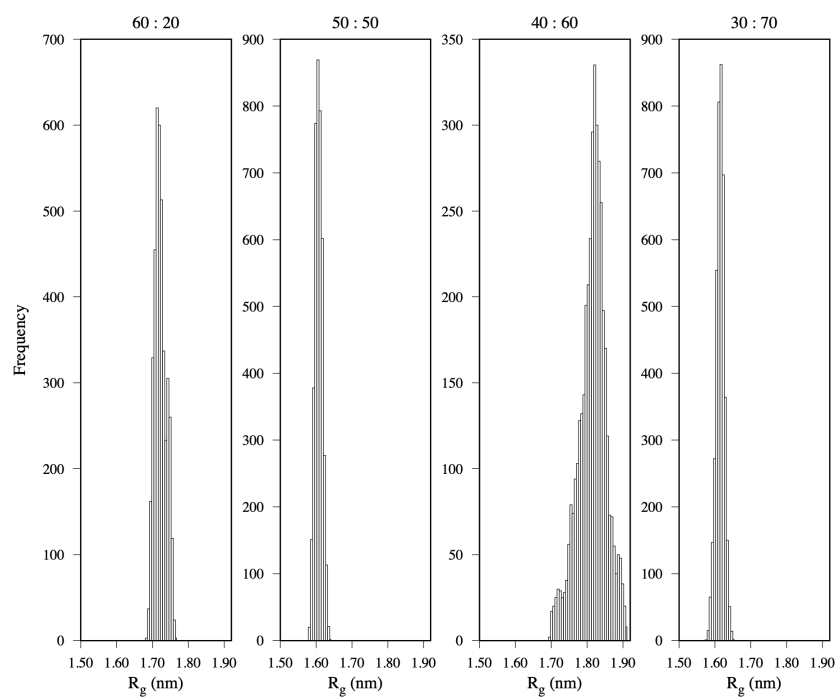
Figure S1: Atom identification in the glycerol molecule.

Density, ρ of glycerol (x_1) : water (x_2) mixtures at 298.15 K and atmospheric pressure.

| $x_1 : x_2$ | Calculated ρ (g/cm ³) | Experimental ρ (g/cm ³) |
|-------------|--|--|
| 100 : 00 | 1.259 \pm 0.002 | 1.25791 |
| 90 : 10 | 1.253 \pm 0.003 | 1.25331 |
| 80 : 20 | 1.250 \pm 0.002 | 1.24648 |
| 70 : 30 | 1.230 \pm 0.001 | 1.23632 |
| 60 : 40 | 1.202 \pm 0.002 | 1.22565 |
| 50 : 50 | 1.174 \pm 0.002 | 1.21375 |
| 40 : 60 | 1.146 \pm 0.001 | 1.19845 |
| 30 : 70 | 1.119 \pm 0.002 | 1.18300 |
| 20 : 80 | 1.091 \pm 0.002 | 1.14286 |
| 10 : 90 | 1.063 \pm 0.002 | 1.09524 |

Histogram of Radius of gyration of the domain in glycerol solutions.





Comparison of cluster sizes of the protein domain: Average distance between clusters within solvents, d_s (nm) and Average distance to centroid, d_c (nm)

| $x_1 : x_2$ | d_s (nm) | d_c (nm) |
|-------------|-------------------|-------------------|
| 100 : 00 | 0.083 ± 0.002 | 0.103 ± 0.004 |
| 90 : 10 | 0.096 ± 0.004 | 0.143 ± 0.008 |
| 80 : 20 | 0.110 ± 0.002 | 0.157 ± 0.010 |
| 70 : 30 | 0.146 ± 0.066 | 0.214 ± 0.008 |
| 60 : 40 | 0.018 ± 0.012 | 0.283 ± 0.011 |
| 50 : 50 | 0.171 ± 0.009 | 0.262 ± 0.010 |
| 40 : 60 | 0.241 ± 0.020 | 0.393 ± 0.023 |
| 30 : 70 | 0.184 ± 0.006 | 0.262 ± 0.016 |
| 20 : 80 | 0.192 ± 0.009 | 0.264 ± 0.012 |
| 10 : 90 | 0.200 ± 0.026 | 0.281 ± 0.020 |

Table S1: Averages of the structural property evaluation of the domain: Root-mean-squared deviation, $RMSD$, Radius of gyration, R_g , Hydrodynamic radius R_{hyd} , End-to-end distance R_{e-e} , and Solvent-accessible surface area, $SASA$.

| $x_1 : x_2$ | $RMSD$ (nm) | R_g (nm) | R_{hyd} (nm) | R_g/R_{hyd} | R_{e-e} (nm) | $SASA$ (nm ²) |
|-------------|------------------|------------------|-----------------|---------------|-----------------|---------------------------|
| 100:00 | 0.41 \pm 0.003 | 1.67 \pm 0.004 | 3.35 \pm 0.01 | 0.499 | 2.81 \pm 0.03 | 946.36 \pm 30.53 |
| 90:00 | 0.45 \pm 0.01 | 1.70 \pm 0.01 | 3.38 \pm 0.01 | 0.503 | 2.69 \pm 0.05 | 963.39 \pm 6.46 |
| 80:00 | 0.48 \pm 0.01 | 1.66 \pm 0.01 | 3.32 \pm 0.01 | 0.500 | 2.34 \pm 0.21 | 929.85 \pm 36.53 |
| 70:00 | 0.59 \pm 0.02 | 1.76 \pm 0.01 | 3.37 \pm 0.01 | 0.522 | 3.19 \pm 0.15 | 961.55 \pm 27.82 |
| 60:00 | 0.64 \pm 0.03 | 1.72 \pm 0.02 | 3.34 \pm 0.01 | 0.515 | 2.70 \pm 0.30 | 930.23 \pm 56.27 |
| 50:00 | 0.63 \pm 0.02 | 1.61 \pm 0.01 | 3.23 \pm 0.01 | 0.498 | 3.62 \pm 0.31 | 837.14 \pm 40.42 |
| 40:00 | 0.88 \pm 0.07 | 1.81 \pm 0.04 | 3.40 \pm 0.02 | 0.532 | 3.08 \pm 0.54 | 891.02 \pm 76.75 |
| 30:00 | 0.48 \pm 0.02 | 1.61 \pm 0.01 | 3.19 \pm 0.02 | 0.505 | 2.24 \pm 0.09 | 796.71 \pm 32.75 |
| 20:00 | 0.76 \pm 0.02 | 1.54 \pm 0.01 | 3.08 \pm 0.01 | 0.500 | 2.51 \pm 0.10 | 759.11 \pm 66.75 |
| 10:00 | 0.68 \pm 0.03 | 1.64 \pm 0.02 | 3.16 \pm 0.02 | 0.519 | 1.95 \pm 0.37 | 758.29 \pm 39.41 |
| 6QHG | 0.00 | 1.51 | 2.91 | 0.519 | 2.28 | 673.71 |