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Research article

Thermal-induced unfolding-refolding of a nucleocapsid COVN protein

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Appendix

Few representative snapshots shows the effect of temperature on folding.

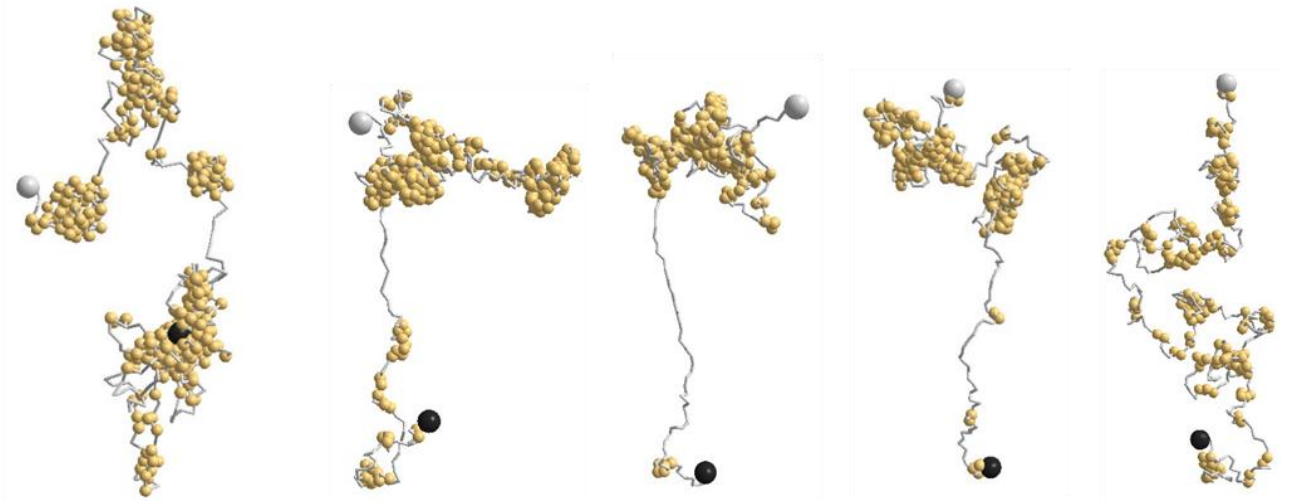

Figure S1. Snapshots of the protein conformation at time step 10^7 at representative temperatures *T=0.0150*, *T = 0.0200*, *T = 0.0230* (first maximum R_g), *T= 0.0240* (minimum R_g), (vii) *T = 0.0268* (second maximum R_g) from left to right. Gold spheres represent residues in contact, the large black sphere is the first residue ^{1}M and large grey sphere is the last ^{422}A.

Details of contact map presented in figures S2 (for entire protein) shows how the degree of folding in different segments in native phase (*T=0.0150*) decreases with unfolding on raising the temperature. For example, the degree of folding in segments ^{118}P–^{164}Q and ^{276}G–^{344}G reduces dramatically by increasing the temperature *T = 0.0150 – 0.0230* as the protein chain denatures to its maxiumum extension (*T=0.0230*). Further heating (*T=0.0230 – 0.0246*) leads to eradicating a large fraction of these folds while the remaining folds in specific segments e.g. ^{62}K –^{70}G, ^{81}P–^{114}L, ^{226}T–^{239}A, ^{248}T–^{270}N, ^{367}T–^{380}A appear to induce contraction in spread of the protein. The degree of folding reduced on continued heating but the persistence of some folded segments e.g. ^{367}T–^{380}A (along with other segments with comparably low folds) lead to futher expansion of the protein (*T=0.0268*) before it reaches to a stable conformation.

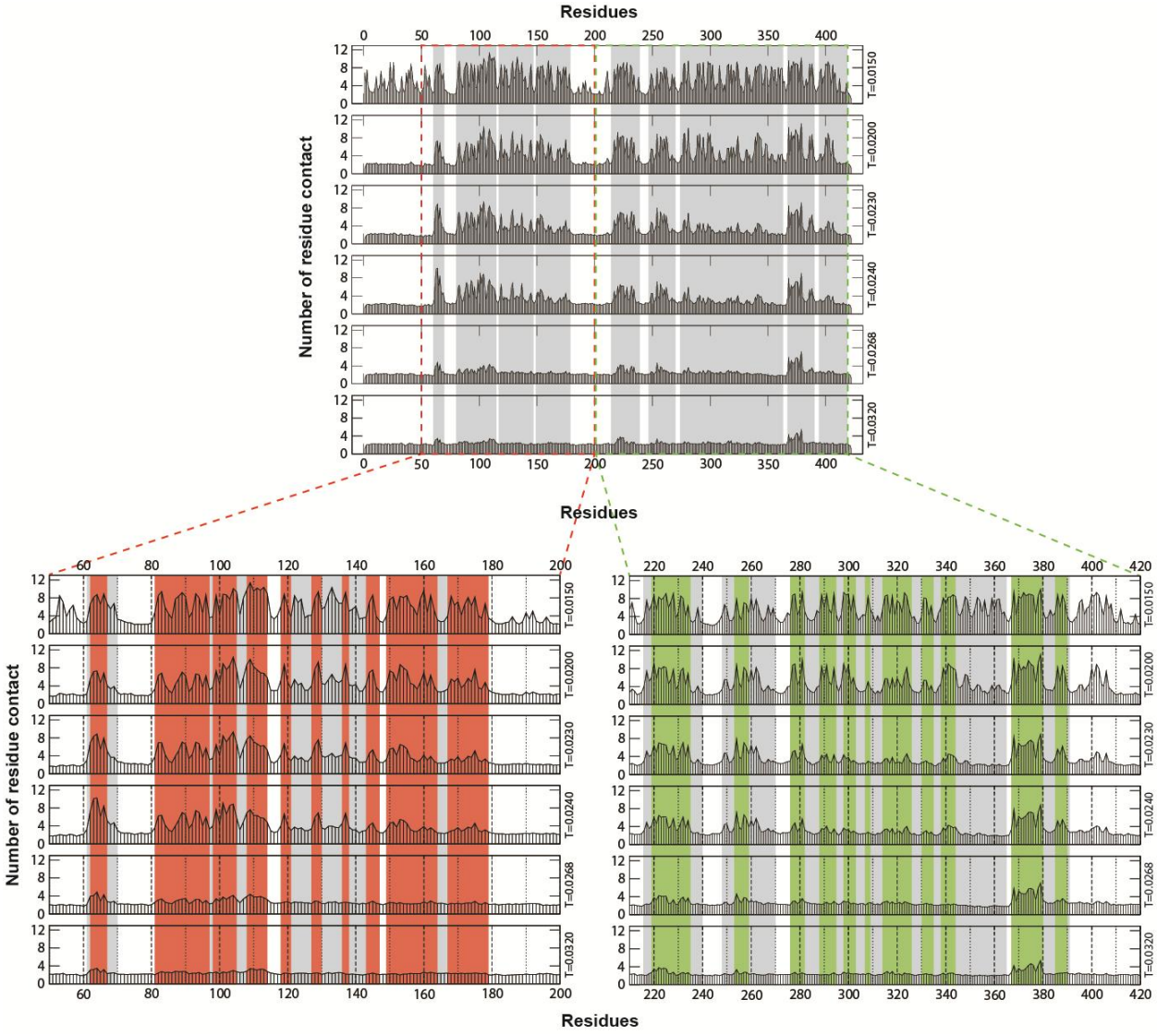

Figure S2. Average number N_n contacts of each residue at representative temperatures *T=0.0150 – 0.032*.

Following segments of COVN with relatively high degree of folding are:

Sequences in left figure: ^{62}K–^{67}F, ^{81}P–^{97}G, ^{98}G–^{105}L, ^{108}R–^{114}L, ^{118}P–^{121}S, ^{127}N–^{130}G, ^{136}T–^{138}G, ^{143}P–^{147}I, ^{149}T–^{164}Q, ^{167}T–^{179}G. Sequences in right figure: ^{219}E–^{235}A, ^{253}A–^{259}P, ^{276}G–^{282}Q, ^{288}G–^{295}Q, ^{298}D–^{303}P, ^{307}Q–^{309}A, ^{314}A–^{326}T, ^{330}T–^{335}H, ^{338}I–^{344}D, ^{367}T–^{380}A, ^{385}Q–^{390}Q, ^{399}A–^{408}L

Note that the folding remains around some segments, e.g. ^{367}T–^{380}A even at high temperature.