Crowding Effects on Amyloid Aggregation Kinetics

Supplementary Materials

Andrea Magno[1], Amedeo Caflisch[1*], and Riccardo Pellarin[1*]

[1] *Department of Biochemistry, University of Zürich, Winterthurerstrasse 190, CH-8057, Zürich, Switzerland*

[*] Authors to whom correspondence should be addressed: caflisch@bioc.uzh.ch, pellarin@bioc.uzh.ch

dE (kcal/mol)	Nucleus size	β-Subdomain size
-2.5	35	18
-2.25	23	10
-2.0	17	17
-1.5	4	4

TABLE 1: The second column lists the number of peptide monomers in the nucleus for different values of the amyloidogenicity dE. The β-subdomain size is the number of monomers in β conformation within the nucleus. The nucleus is defined as the aggregate with 50% probability to further evolve into a fibril and 50% probability to dissolve into isolated monomers.

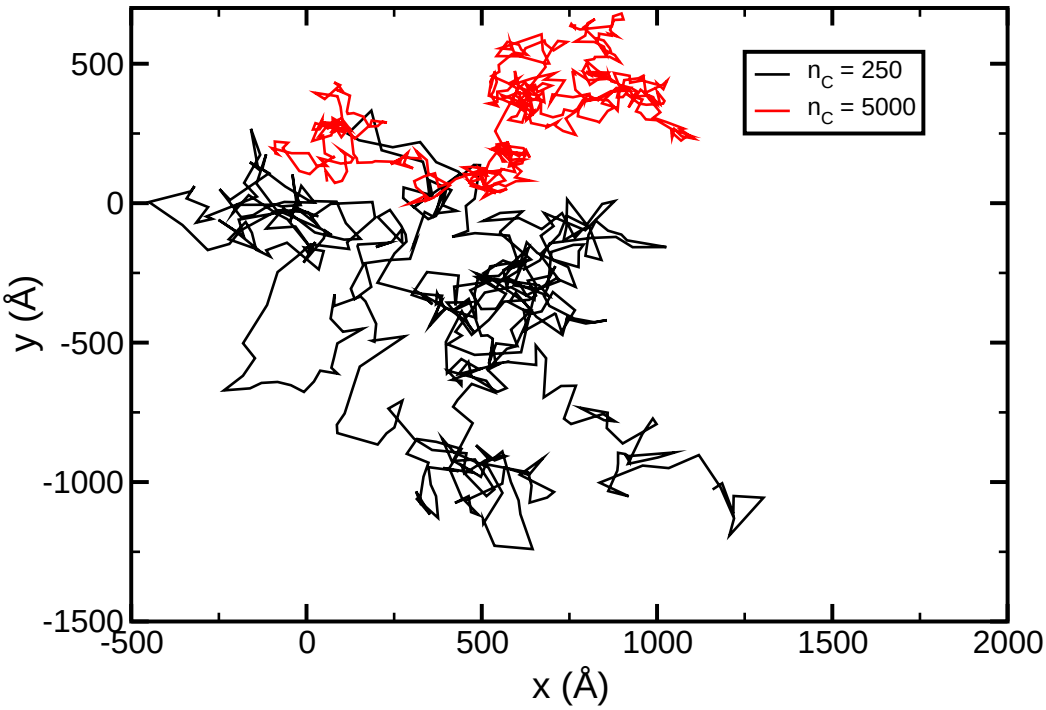

FIG. 1: Projection on the $x-y$ plane of a 20 ns-long trajectory of a peptide at different crowders concentration. The projection shows that at high concentration of crowders the motion of the peptide is hindered.

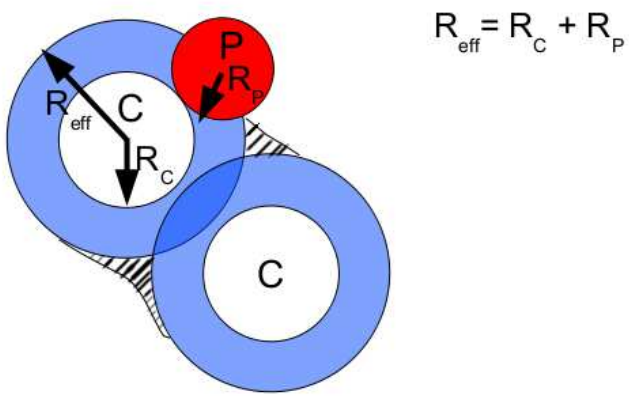

FIG. 2: Effective volume excluded to a peptide (P) by two crowders (C). Since the radius of the peptide is non-negligible with respect to the one of the crowder, the excluded volume evaluation requires two corrections. The first correction accounts for the overlying volume between crowders (darker blue area), and the second derives from the interstitial volume between two or more crowders which is inaccessible to the peptides (shaded area).

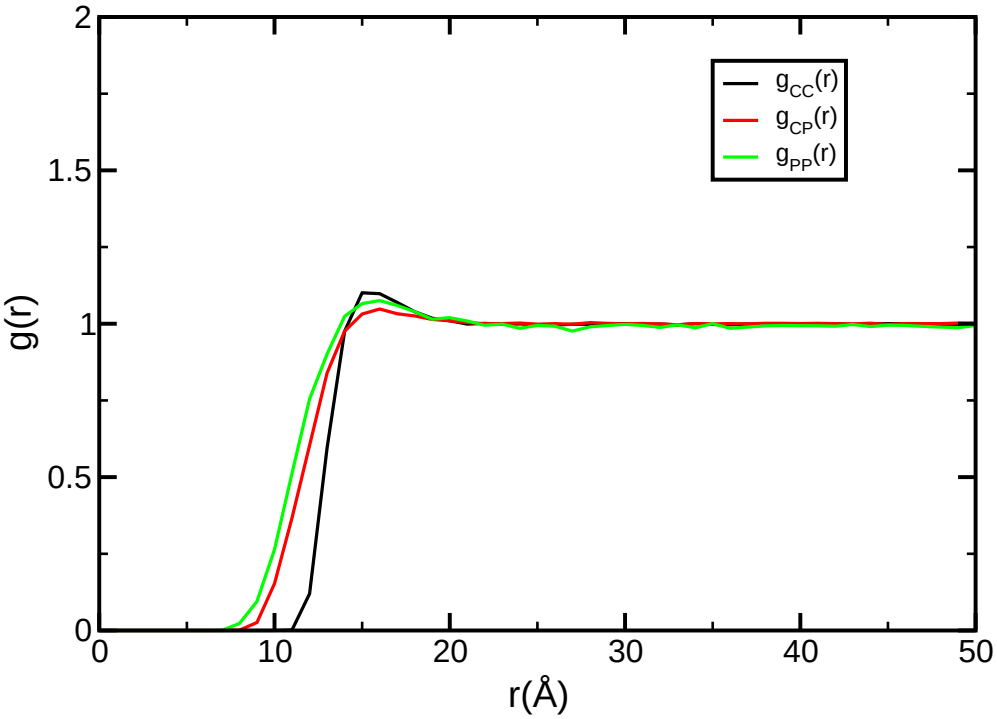

FIG. 3: Radial distribution functions of each pairs of species present in the solution (C=crowder, P=peptide).

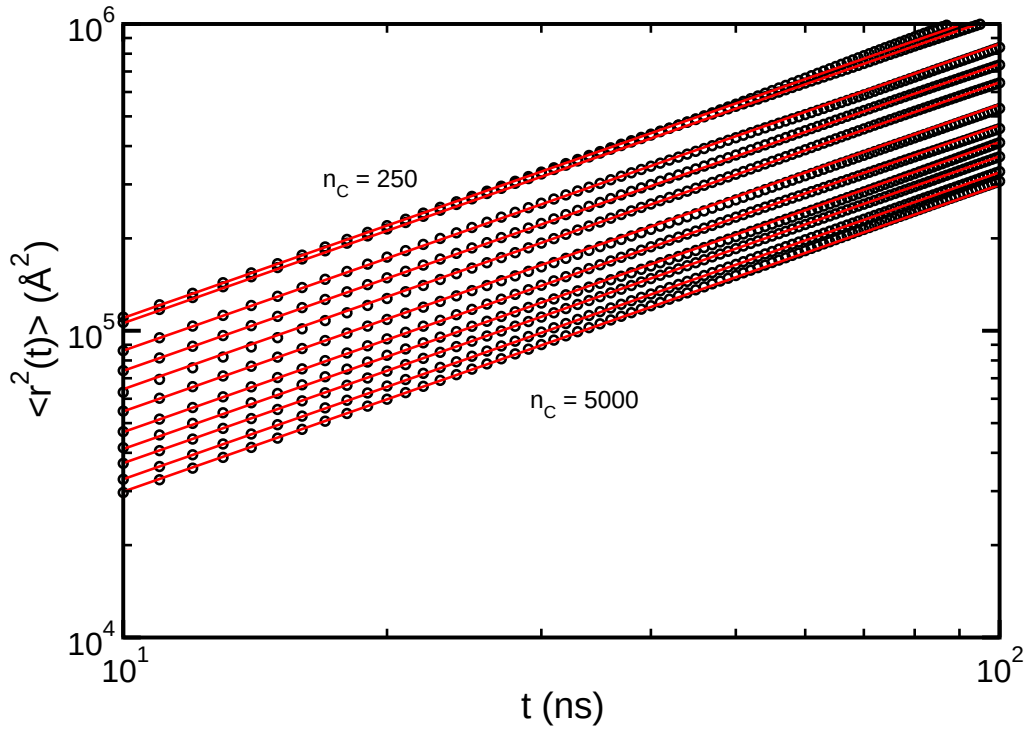

FIG. 4: Long time behaviour of the peptide mean square displacement $\langle r^2(t)\rangle$ (black circles) derived from the trajectories and linear fit with Einstein's relation (red lines) at different crowder content.