

SUPPLEMENTARY MATERIAL

FIGURE S1. Outcome of the constrained modelling analyses of the MBL oligomers.

The R -factor values for the 900-6,859 trial models of the MBL oligomers are compared with the corresponding R_G values. The parameters for all the models are shown as open yellow circles. The vertical dashed lines correspond to the experimental R_G values obtained from the Guinier fit (black) and the $P(r)$ analyses (blue). In all four panels the 10-12 best models are represented by blue circles (Tables 2 and 3). The best-fit model from each search is shown in red (Tables 2 and 3).

A, Fit search 1 for the MBL monomer, based on the swivel region. For this, the 5,000 models were created using a conformationally-randomised 70-DSRAIE-75 linker, starting from the linear MBL monomer model (Figure 5B).

B, Fit search 2 for the MBL dimer. In the starting model, two best-fit MBL monomers were aligned end-to-end, with the Gly29 residues on chain A in each monomer separated by 3.3 nm. In this search, 6,859 rotational models were created by holding monomer 1 stationary and rotating monomer 2 in 19 steps of 10° between 0° and 180° about the X-, Y- and Z-axes.

C, Fit search 2 for the MBL trimer. Three best-fit MBL monomer structures were superimposed upon one another, then 2028 trimer models were created by holding monomer 1 stationary and rotating monomers 2 and 3 at 10° steps between 10° and 120° and between 20° and 240° respectively about the X-, Y- and Z-axes.

D, The fit search for the MBL tetramer. Four best-fit MBL monomer structures were superimposed upon one another, and 900 models were generated by keeping monomer 1 at 0° , 0° , 0° , about the X-, Y- and Z-axes and rotating monomers 2, 3, and 4 at 10° increments between 10° and 90° , 20° and 180° and 30° and 270° , respectively.

FIGURE S2. Superimposition of the randomised and best-fit models of MBL oligomers.

In the eight panels, the best-fit model is shown in pink. The other models are shown in purple, or green. In panels *A*, *C*, *E* and *G*, two orthogonal views are shown, indicated by the labelled arrows. The 10-12 best-fit models from each analysis are provided in Supplementary Material.

A-B, Superimposition of the first 100 of the 5,000 models created in Search 1 for the MBL monomer. The models assessed the relative orientation of the CRD and neck region in relation to the collagen region in panel *A*. The best-fit 12 models from Search 1 are shown in panel *B* (Table 2).

C-D, Every 66th model of the 6,859 models created in Search 2 for the MBL dimer was superimposed for panel *C*. The best-fit 12 models from this search are superimposed onto monomer 1 (at the right) in panel *D*, indicating the range of possible positions for monomer 2.

E-F, Every 36th model of the 2,028 models created in Search 2 for the MBL trimer are superimposed for panel *E*. The 12 best-fit models from this search are superimposed using monomer 1 (at the right) in panel *F*. The conformations of two symmetry-related trimer models are shown in purple and green for clarity.

G-H, Every 18th model of the 900 created in the MBL tetramer search are superimposed in panel *G*. The best-fit 10 models were superimposed using monomer 1 (at the left) in panel *H*.

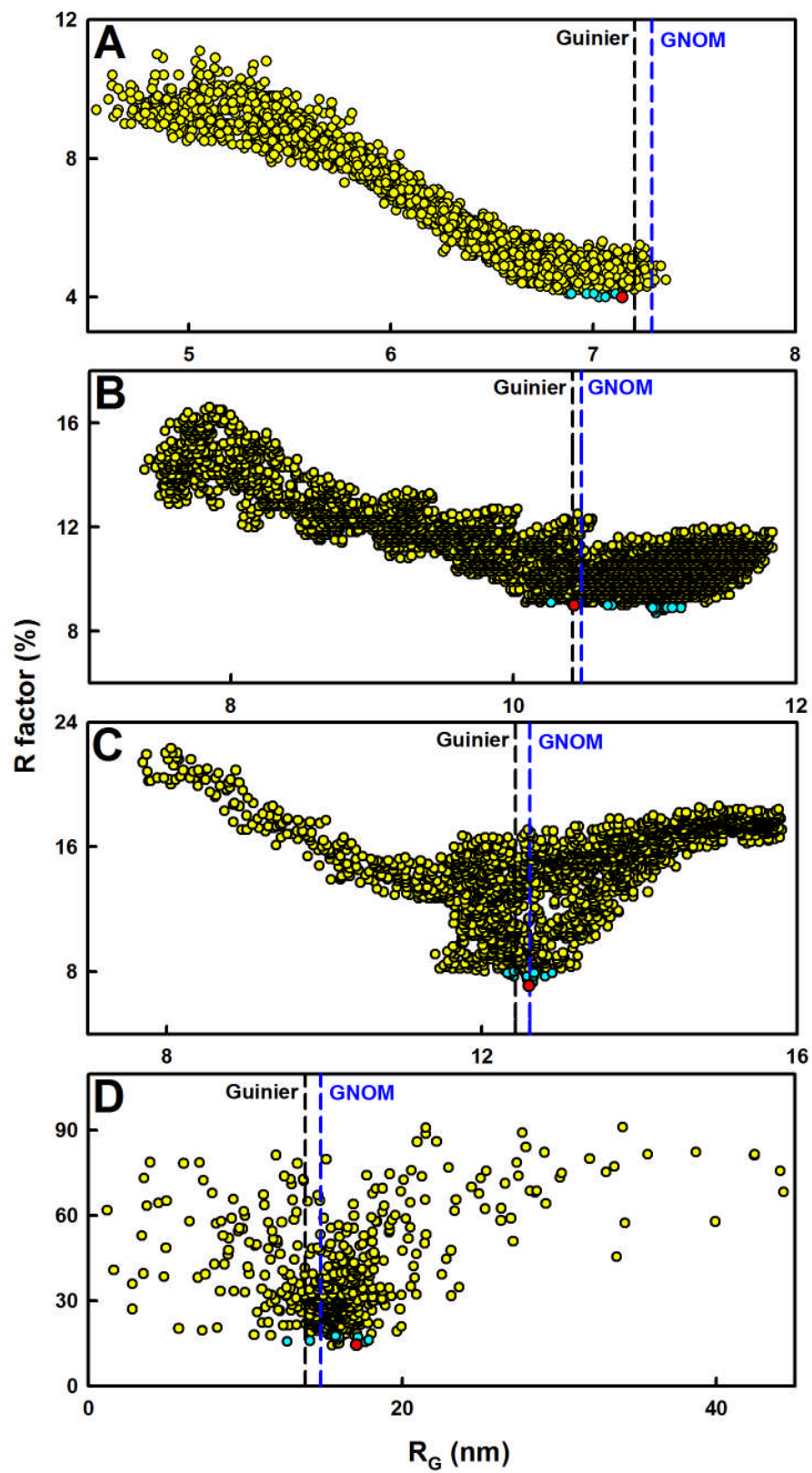


Figure S1

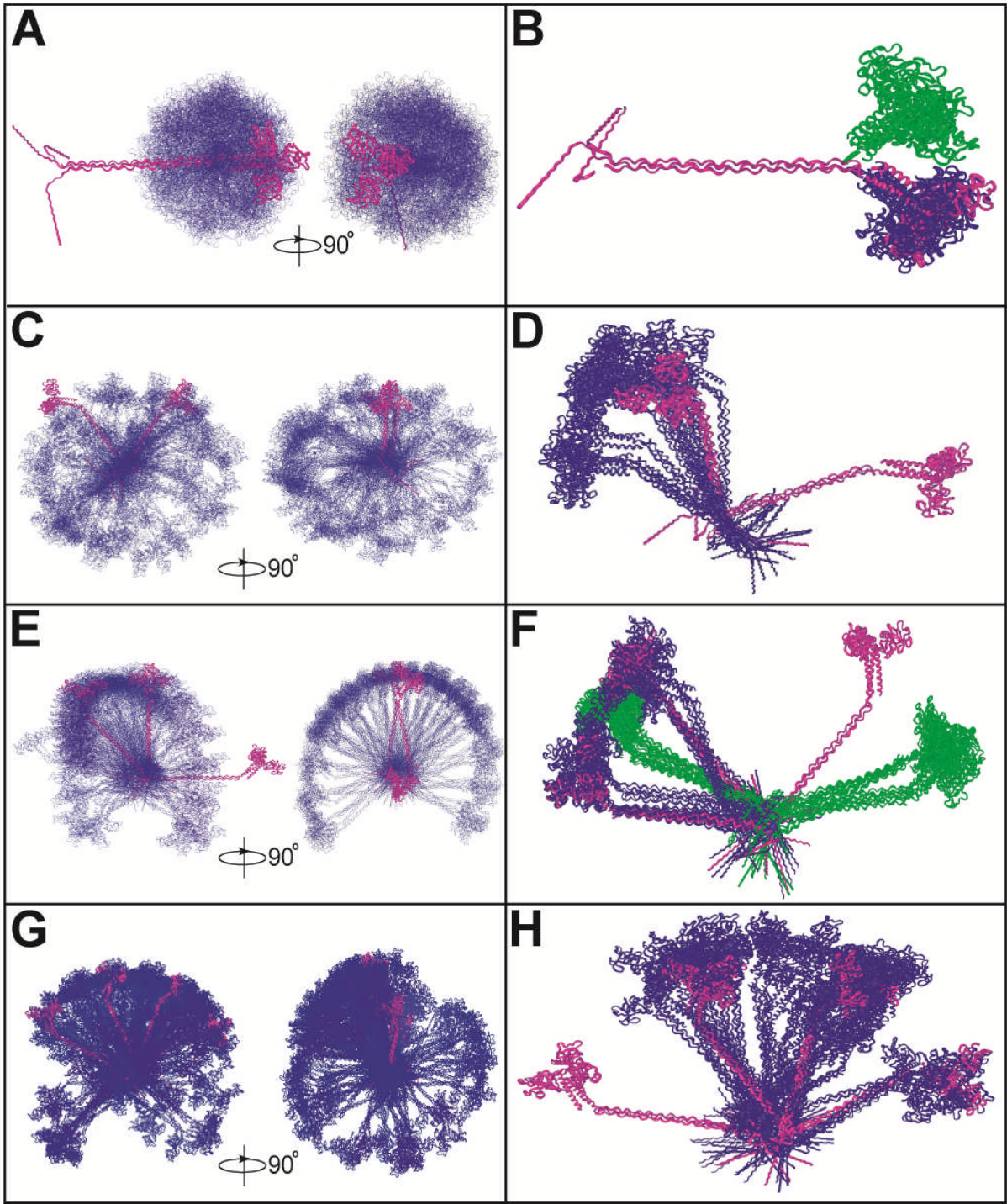


Figure S2