

ARTICLE TYPE

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## Electronic supplementary information: Temperature induced conformational changes in the elastin-like Peptide GVG(VPGVG)<sub>3</sub>

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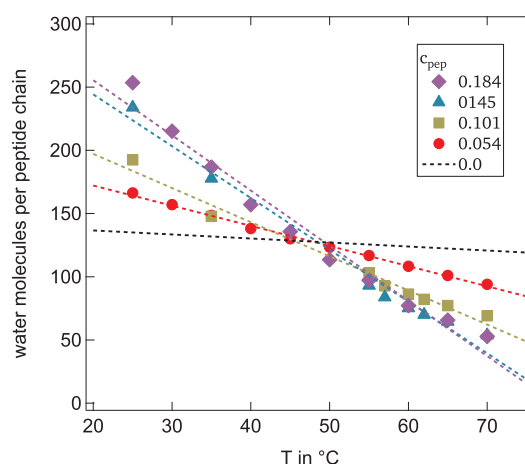
### 1 Details on the scattering constant

The fitting model given in equation 1 of the main article includes the pre-factor  $c$ , which is given by  $c = c_m \cdot K \cdot M_1$ . The pre-factor depends on the mass concentration  $c_m$  of peptide in the buffer, the scattering constant  $K$  and the molecular weight  $M_1$  of the scattering object, i.e. the hydrated peptide.<sup>1,2</sup> Decomposing the scattering constant further we obtain

$$K = (\Delta\rho_{\text{SLD}})^2 \frac{v_1^2}{M_1^2 N_A}, \quad (1)$$

including the molar volume of the scattering object  $v_1$ , Avogadro's Number  $N_A$  and the contrast in scattering length densities  $\Delta\rho_{\text{SLD}}$  between the buffer solution and the hydrated peptide. Since the hydration number of the peptide ( $n_{\text{hyd}}$  = number of water molecules per peptide chain) is not known it is treated as a fitting parameter. However, the precise value of  $n_{\text{hyd}}$  depends crucially on the peptide's molar volume, explicitly included in equation 1 of the ESI and implicitly in  $\Delta\rho_{\text{SLD}}$ , which can be only estimated. Based on the mass density of PEG of 1.13 g/cm<sup>3</sup> we assume the molar volume of the peptide to be  $v_1 = 1300 \text{ cm}^3/\text{mol}$  within 10% accuracy.<sup>3</sup> The resulting hydration numbers for all investigated peptide concentrations and temperatures are given in figure 1 of the ESI.

As can be seen the hydration number is systematically decreasing with increasing temperature. This observation is in accordance with the increasing intensity of the low  $q$ -value plateau depicted in the upper panel of figure 1 of the main article. If water is expelled from the scattering peptide the scattering length density difference between hydrated peptide and surrounding buffer solution increases leading to stronger scattering at small  $q$ -values. Furthermore, it supports our interpretation of an aggregation process upon heating, favouring peptide-peptide interaction above water-peptide interactions. For each investigated concentration the hydration number decreases linearly with tem-



**Fig. 1** Hydration numbers for all investigated peptide concentrations and temperatures deduced from fitting of the pre-factor given in equation 1 of the main article.

perature. Extrapolating this linear dependency to zero concentration the dashed black line depicted in figure 1 is obtained. The slope of this extrapolated line is  $(-0.3 \pm 0.1) \text{ K}^{-1}$  which is in agreement with molecular dynamic simulations on an isolated GVG(VPGVG)<sub>3</sub> chain.<sup>4</sup> However, absolute values have to be treated with caution, due to the 10% uncertainty in the peptide's molar volume, given hydration numbers may be  $\pm 50\%$  off.

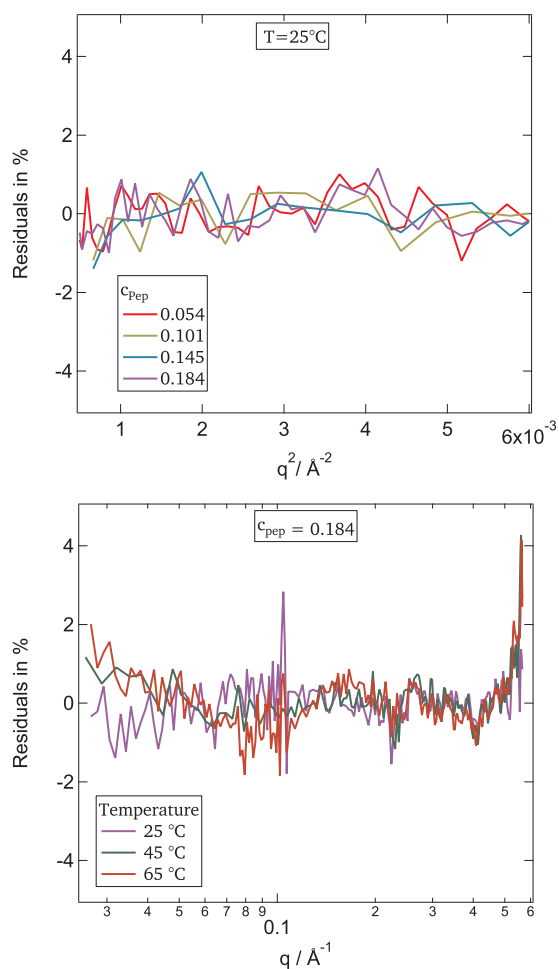
### 2 Residual plots

In the main article fitting by either the Guinier approach or the model function given in equation 1 is performed. For the two datasets presented in figure 2 and 7 of the main article we depict here in figure 2 the respective residual plots. For the Guinier approach fit accuracy is very good all deviations are below 1% along the whole range of considered  $q$ -values. Fitting the high concentration sample at various temperatures with the more complex model given in equation 1 of the main article, shows slightly more deviations. However, fitting accuracy is still better than 2%.

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**Fig. 2** Residual plot for the fitted datasets presented in figure 2 (upper panel) and 7 (lower panel) of the main article.

## References

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