Electronic Supplementary Information belonging to the manuscript:

Solution scattering studies on a virus capsid protein as a building block for nanoscale assemblies

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Effect of D_2O on virus and capsid

As described in the Introduction, the presence of D_2O improves the contrast and therefore the information obtained from the SANS data. In order to be able to perform the SANS studies properly, it was felt necessary to study the influence of D_2O on the assembly behavior of CCMV and the CCMV capsid. The effect of D_2O was studied by FPLC and the results are shown in Figure S1. In the case of the CP (Figure S1a and b), the samples eluted at exactly the same time, which shows that the change from hydrogen to deuterium does not really affect the structure of the particles. However, in the case of the virus (Figure S1c and d), we observed that the D_2O solutions tended to elute later, although the difference was small. The appearance of the particles in TEM appeared not to be affected (not shown). The delayed elution would suggest a decrease in particle size in D_2O, but this is not confirmed with the SANS studies.

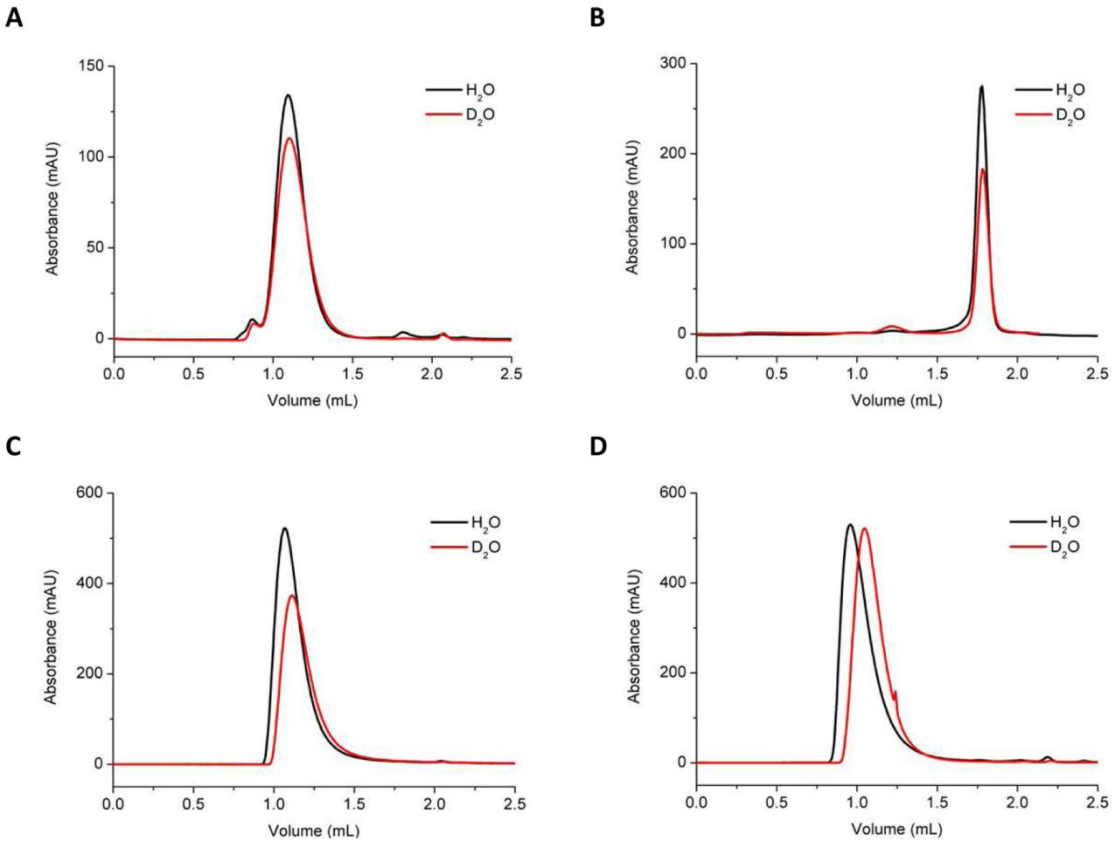


Figure S1. FPLC chromatograms of CCMV CP at a) pH/pD 5 and b) pH/pD 7.5, and CCMV at c) pH/pD 5 and d) pH/pD 7.5, showing traces for both H_2O and D_2O solutions. The samples containing capsid protein contained 1 M NaCl whereas those containing CCMV contained no NaCl.

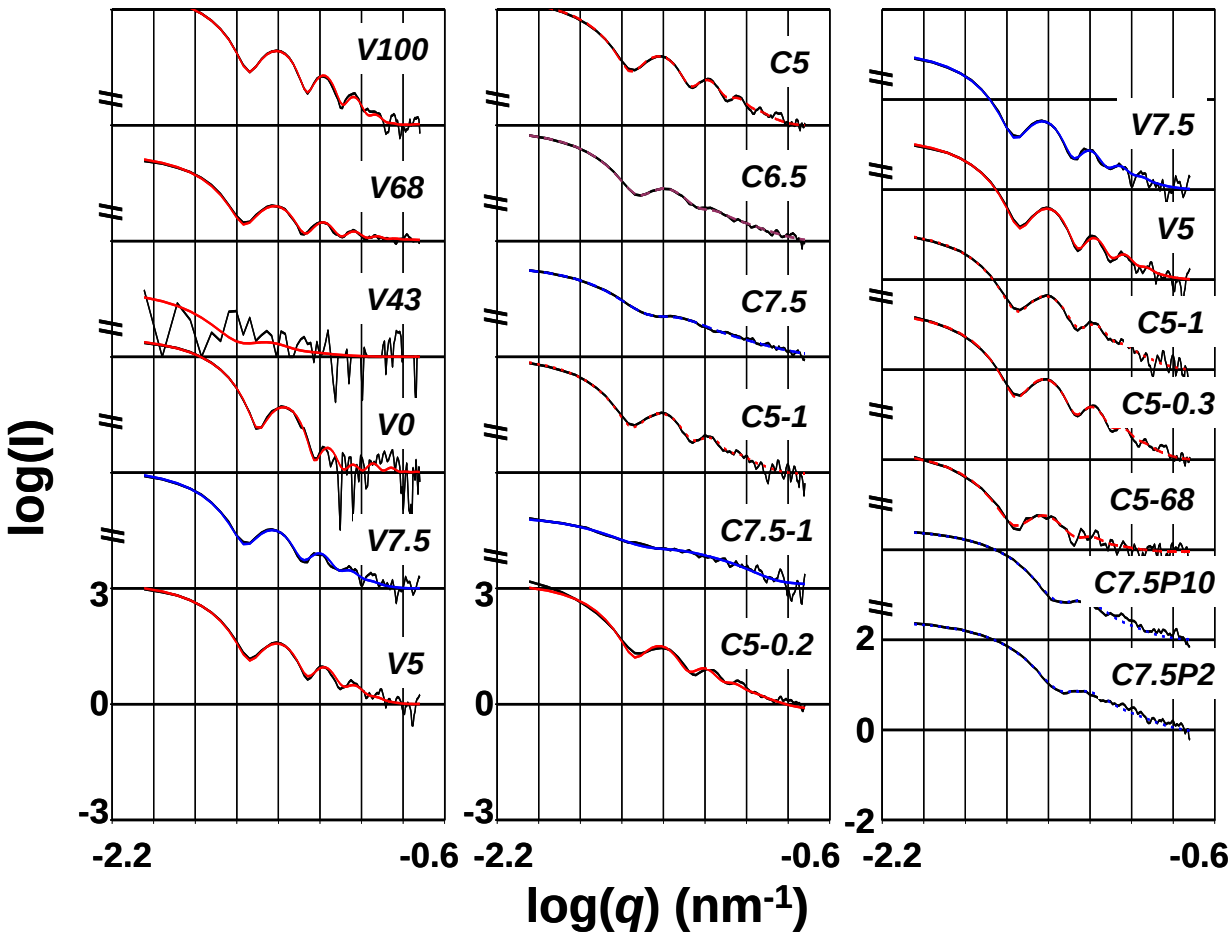
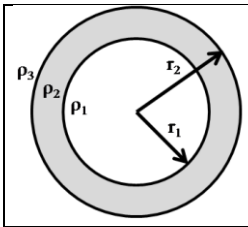


Figure S2. SANS simulations of Figure 5 in the manuscript, represented as log(I) vs log(q). SANS curves (solid black, experimental; solid colours, fits with the parameters given for the corresponding labels (e.g. *V100*) in Tables 1 (core-shell, left and middle panel) and 2 (core-2 shell, right panel)). Left panel, CCMV with varying contrast (D_2O/H_2O v/v) and pD; middle panel, CCMV CP at various pDs and ionic strengths; right panel, core 2-shell fits of CCMV and capsid with and without polymer. See Tables 1 and 2 (manuscript) for the meaning of the labels. Fits at pD 5, pH 6.5, and 7.5 have been depicted with red, violet, and blue traces respectively, throughout the Figure.

Additional SANS simulation parameters. For a number of SANS samples where CP dimers are in equilibrium with empty capsids fits of a quality equivalent to (C6.5-0.3, C7.5-0.3) or identical with (C7.5-1) the fits shown in Figure 4 could be obtained when a disc component was included to simulate a contribution of capsid protein dimers; the parameters are given in Table S1.

Table S1. Parameters for fits with core–shell model component (r, radius (nm); ρ, contrast (scattering length density, 10^{-14} cm Å^{-3}); PD, ((standard deviation)/mean of r_2, %) and a protein disc component (r, radius (nm); l, thickness (nm)) of SANS data obtained from experiments with CCMV CP at various pD values and ionic strengths. Labels C6.5-0.3, C7.5-0.3, and C7.5-1 refer to the experimental traces in Figure 3 (middle panel). Top left corner: schematic representation of the core-shell model (see also Figure 3).

		$\rho_1-\rho_2$	r_1 (nm)	Δr (nm)	r_2 (nm)	$\rho_2-\rho_3$ (fixed)	PD (%)	r_{disc} (nm)	l_{disc} (nm)
C6.5-0.3	pD 6.5, 0.3 M	3.25	8.82	2.71	11.53	−3.25	13.24	3.0	2.8
C7.5-0.3	pD 7.5, 0.3 M	3.25	6.71	3.27	9.98	−3.25	17.00	2.4	2.8
C7.5-1	pD 7.5, 1 M	3.25	6.48	2.80	9.28	−3.25	17.00	2.9	2.8

SANS simulations with scattering length density gradients. The simulation programme FISH allows for adaptations of the core-shell model with an *r*-dependent profile in which the scattering length density varies gradually with *r*.

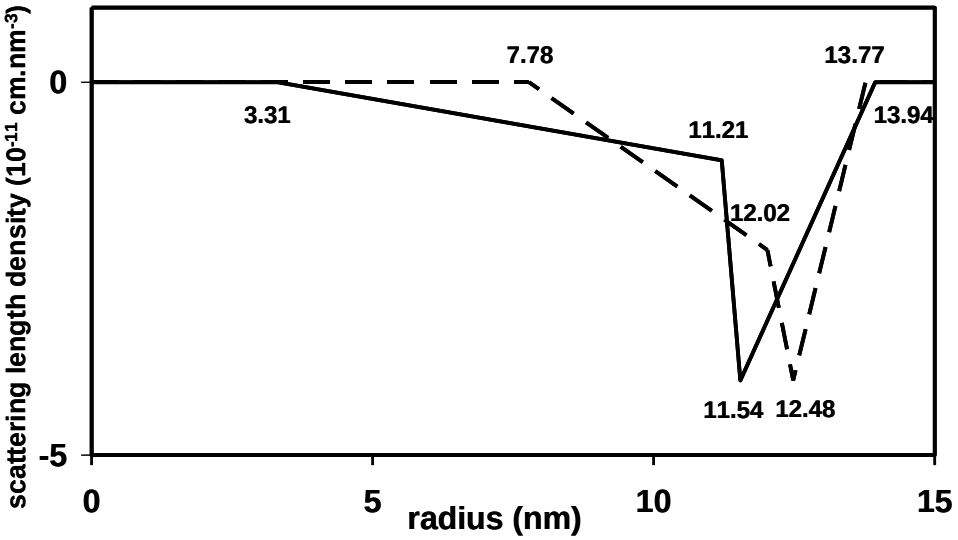


Figure S3. *r*-dependent profiles for simulations with gradually varying scattering length density of CCMV (solid) and capsid protein (at 0.3 M NaCl, dashed) in D_2O, pD 5.0, giving fits of equivalent quality to the ones included (entries *V5* and *C5-0.3*) in Figure 5. The numbers represent the values of *r* at the turning points.

Table S2. Buffer conditions used for the different virus and capsid samples.

Samples	Buffer conditions[a)]		
Virus pH 5	50 mM sodium acetate		
Virus pH 7.5	50 mM Tris-HCl		
Capsid pH 5	50 mM sodium acetate 200 mM NaCl	50 mM sodium acetate 300 mM NaCl	50 mM sodium acetate 1 M NaCl
Capsid pH 6.5		50 mM ammonium acetate 300 mM NaCl	
Capsid pH 7.5		50 mM Tris-HCl 300 mM NaCl	50 mM Tris-HCl 1 M NaCl

a) All buffers used in the assembly studies additionally contained 1 mM EDTA, 10 mM $CaCl_2$, and 0.2 mM Phenylmethanesulfonyl fluoride (PMSF).