SUPPLEMENTARY INFORMATION

Disentangling polydispersity in the PCNA–p15^{PAF} complex, a disordered, transient and multivalent macromolecular assembly

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FIGURE S1.

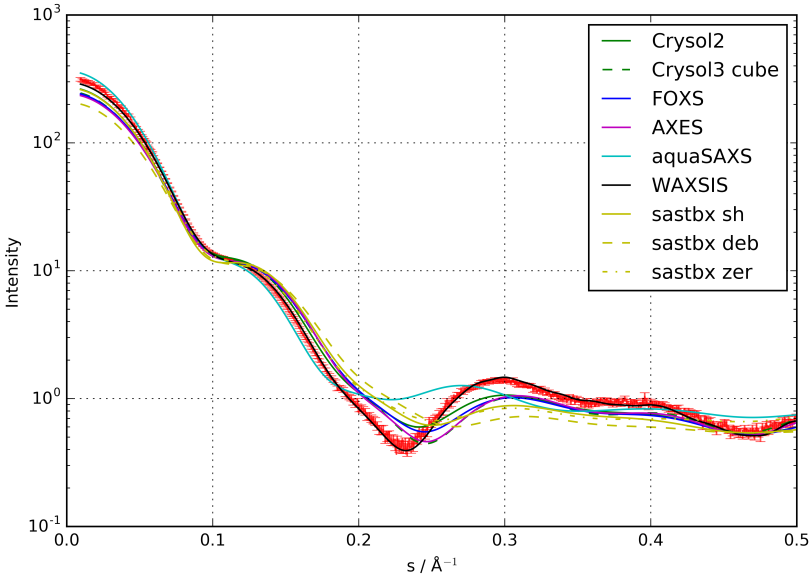

Figure S1. Theoretical SAXS curves for the PCNA computed using different approaches (see references in the main text) compared with the experimental data. Theoretical SAXS profiles were computed directly from the same X-ray structure (PDB code: 4D2G) using the default settings provided by the developers. Final theoretical curves were scaled to achieve the best agreement to the experimental data. Experimental SAXS data displayed as red circles with error bars and the different simulated curves by solid or dashed lines as indicated in the inset. We used the three calculation methods that are available in SASTBX: spherical harmonics (sastbx sh), Debye formula (sastbx deb) and Zernike polynomials (sastbx zer).

FIGURE S2.

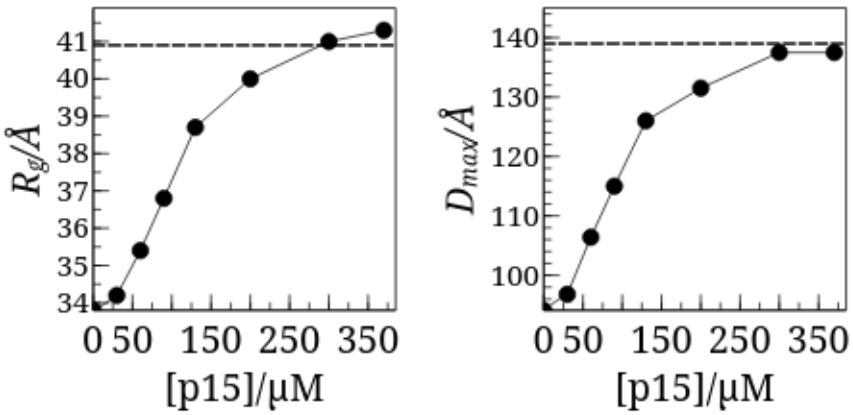

Figure S2. Evolution of R_g and D_{max} values extracted from experimental SAXS titration dataset with respect to p15 concentration. Both parameters were derived from the pair-wise distance distribution function *P(r)*. Dashed lines correspond to the expected values derived from the ensemble corresponding to the 3:3 PCNA-p15 complex

FIGURE S3.

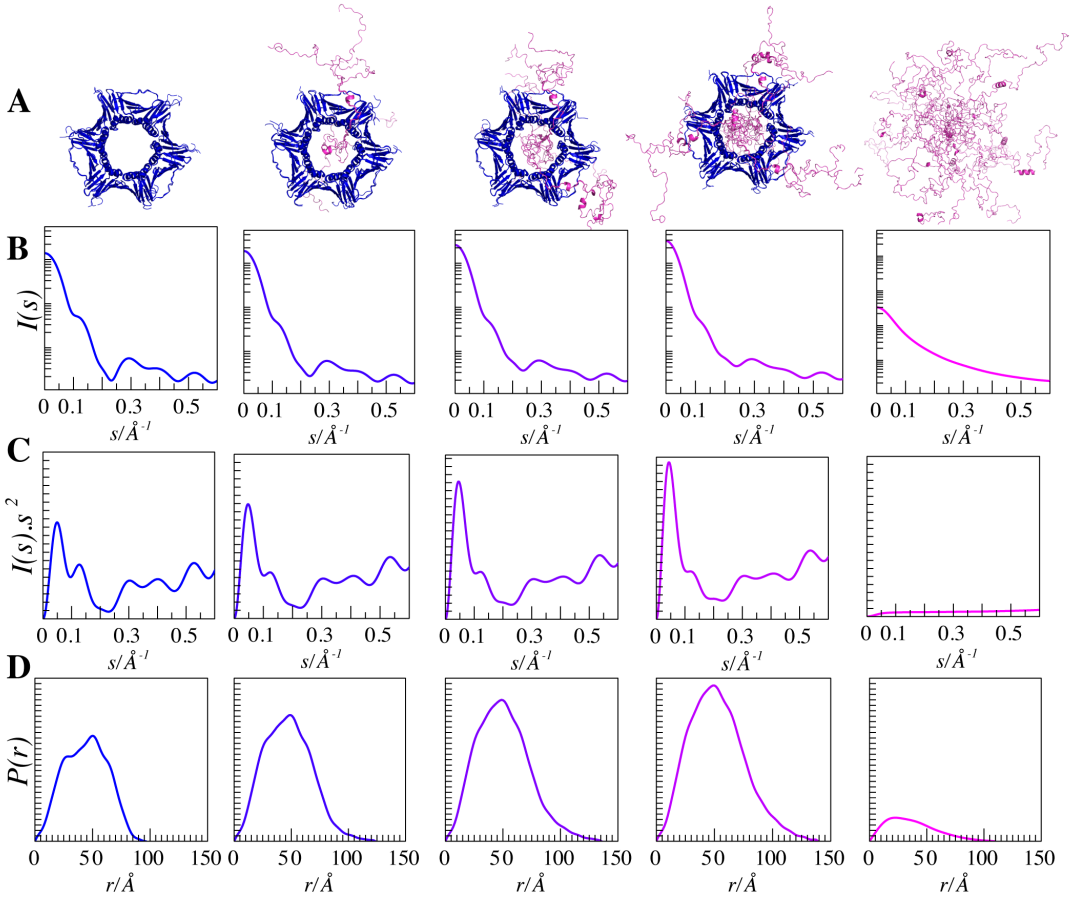

Figure S3. SAXS observables computed form 800 all-atom models for the 5 co-existing species present in mixtures of PCNA and p15 depicted in (A). (B) SAXS profiles, (C) Kratky representations, and (D) *P(r)* functions.

FIGURE S4.

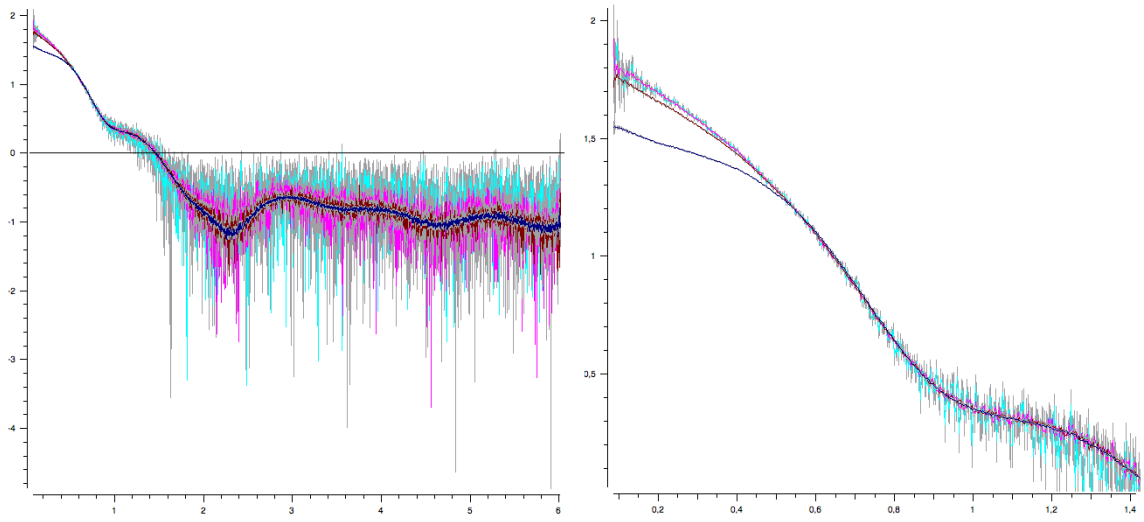

Figure S4. Scattering profiles for PCNA at 1.3 (cyan), 3.0 (pink), 10.6 (brown), and 42.4 (dark blue) mg/ml measured in EMBL X33 beamline at DESY displayed at the full momentum transfer range measured (left) and at the lowest angles (right). The similarity between the curves at 1.3 and 3.0 mg/ml indicates the absence of repulsive interparticle interactions at 3.0 mg/ml.

FIGURE S5.

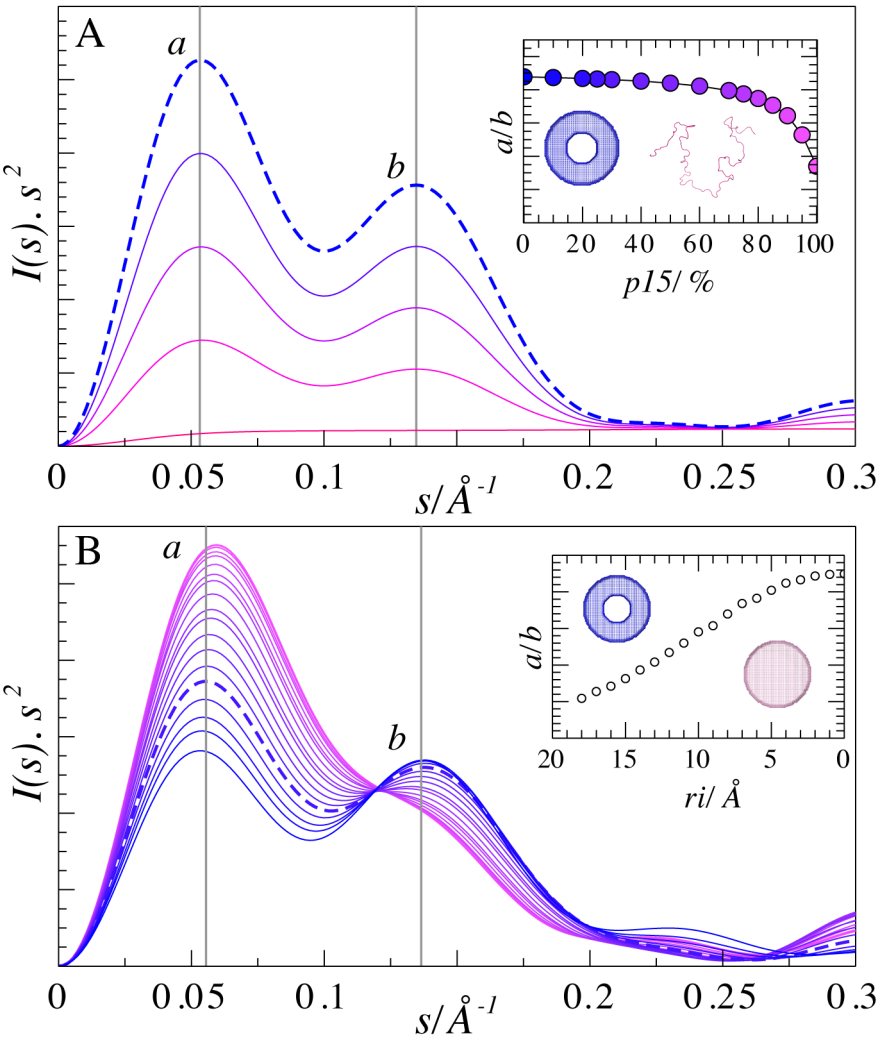

Figure S5. Analysis of SAXS data using geometric models. (A) Kratky representation of mixtures of a hollow cylinder with increasing molar fractions of non-interacting Gaussian chain. Inset: Peak intensity ratios are plotted as function of the relative population of p15 in the mixture. (B) Kratky representation of hollow cylinders with increasing inner ring radius. Inset: Peak intensity ratios are plotted as a function of inner ring radius (*ri*). The dashed-lines correspond to a Kratky plot of a hollow cylinder representation of the same size than PCNA.