

SUPPLEMENTAL DATA

SUPPLEMENTAL FIGURE LEGENDS

Supplemental Fig. 1. SPRS analysis of PCNA binding by homo- or heteroduplex-bound MutS α .

(A) SPRS analysis of PCNA binding to heteroduplex-bound MutS α was performed using a streptavidin sensor chip derivatized with 150 RUs of 201-bp heteroduplex or homoduplex DNA. Flow of 200 nM MutS α was initiated at 300 s. At 600 s MutS α flow was either continued (dashed blue line) or supplanted by flow of a solution containing both 200 nM MutS α and 2.5 μ M PCNA (red line). RU increase due to PCNA binding was estimated from mean values observed in the presence or absence of PCNA from 650 to 1200 s. Mass bound to homoduplex DNA in the presence of MutS α alone (dashed green line) or MutS α supplemented with PCNA at 600s (orange) is also shown. Mass bound to the heteroduplex substrate upon flow of PCNA alone is depicted by the black line. **(B)** Binding isotherm for PCNA binding to the MutS α •DNA complex as determined from experiments like those shown in **panel A**. Molar stoichiometries were calculated as in **Fig. 1C**.

Supplemental Fig. 2. Experimental and calculated SAXS properties of MutS α and PCNA. **(A)**

Experimentally determined scattering profiles (solid lines) (reproduced from **Fig. 4**) are compared with profiles calculated using CRY SOL (1) from crystal structures (dotted) of PCNA (black and grey) (2) and the MutS α Δ 341•DNA complex (dark and light brown) (3). **(B)** Forward scattering intensities $I(0)$ (intensity at $\theta = 0^\circ$) for MutS α , MutS α Δ 12, MutS α Δ 341, PCNA, and a 1:1 mixture of MutS α with the PCNA trimer were determined from concentration-normalized scattering data using the Guinier equation and are plotted versus the molecular weight of each species. **(C)** *Top*, Models shown were generated using the PyMOL program by manually

docking the crystal structures of PCNA (2) and MutS α Δ 341 (3) such that the putative complex is in an extended configuration (left and middle) or in a stacked configuration (right), in which the DNA binding channels of MutS α Δ 341 and PCNA are aligned so as to permit a linear segment of helix to thread through both. The two extended configurations shown differ in the relative orientation of PCNA and MutS α Δ 341 about the y axis (90° relative rotation). *Bottom*, CRYSOLE was used to calculate theoretical solution scattering profiles for MutS α Δ 341, as well as the extended and stacked model complexes shown in the *Top*. These theoretical profiles were used as input to GNOM (4) to generate P[r] plots shown for MutS α Δ 341 (blue line), the two extended (dotted red line and hyphenated green line), or the stacked (dotted blue line) complex.

Supplemental Fig. 3. *Ab initio* shape reconstructions of the MutS α •PCNA complex. (A) Two rotational views of seven independent shape reconstructions of the MutS α •PCNA complex are shown (in addition to views depicted in **Fig. 5**). The crystal structures of MutS α Δ 341 and PCNA were manually docked into the SAXS envelopes (grey spheres).

Supplemental Fig. 4. R_g dependence on protein concentration. Dependence of apparent R_g on protein concentration is shown for MutS α (blue circles), MutS α Δ 12 (green circles), MutS α Δ 341 (red circles), MutS α Δ 341•DNA complex (brown circles), PCNA (black circles), and the MutS α •PCNA complex (orange squares). MutS α , MutS α Δ 12 and MutS α •PCNA exhibited a low level of interparticle interaction.

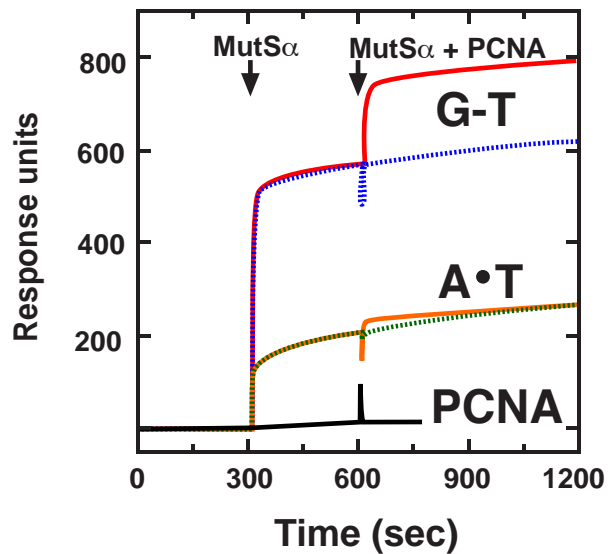
SUPPLEMENTAL REFERENCES

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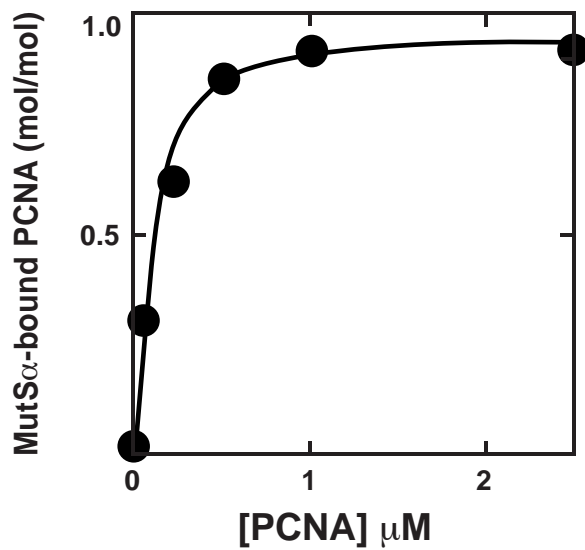
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Supplemental Fig. 1

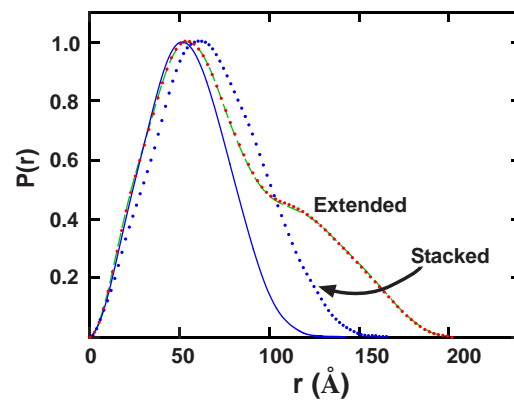
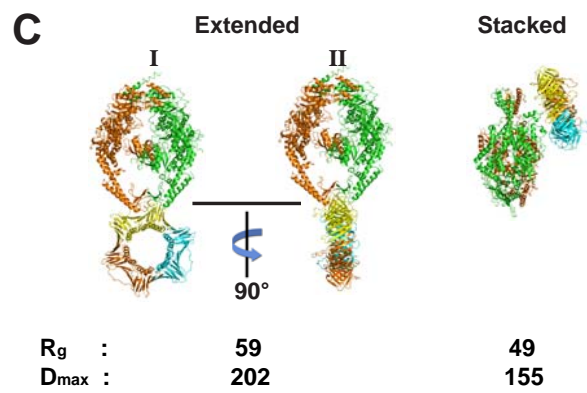
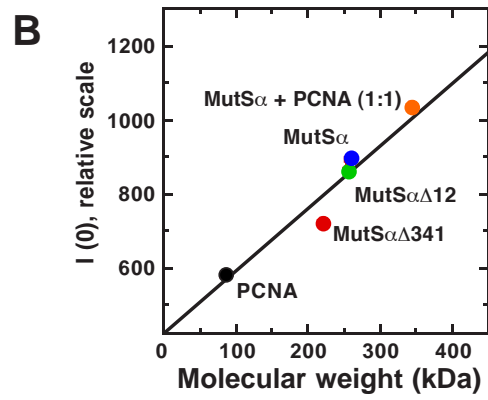
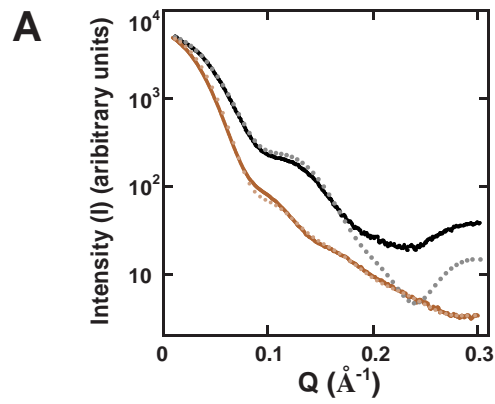
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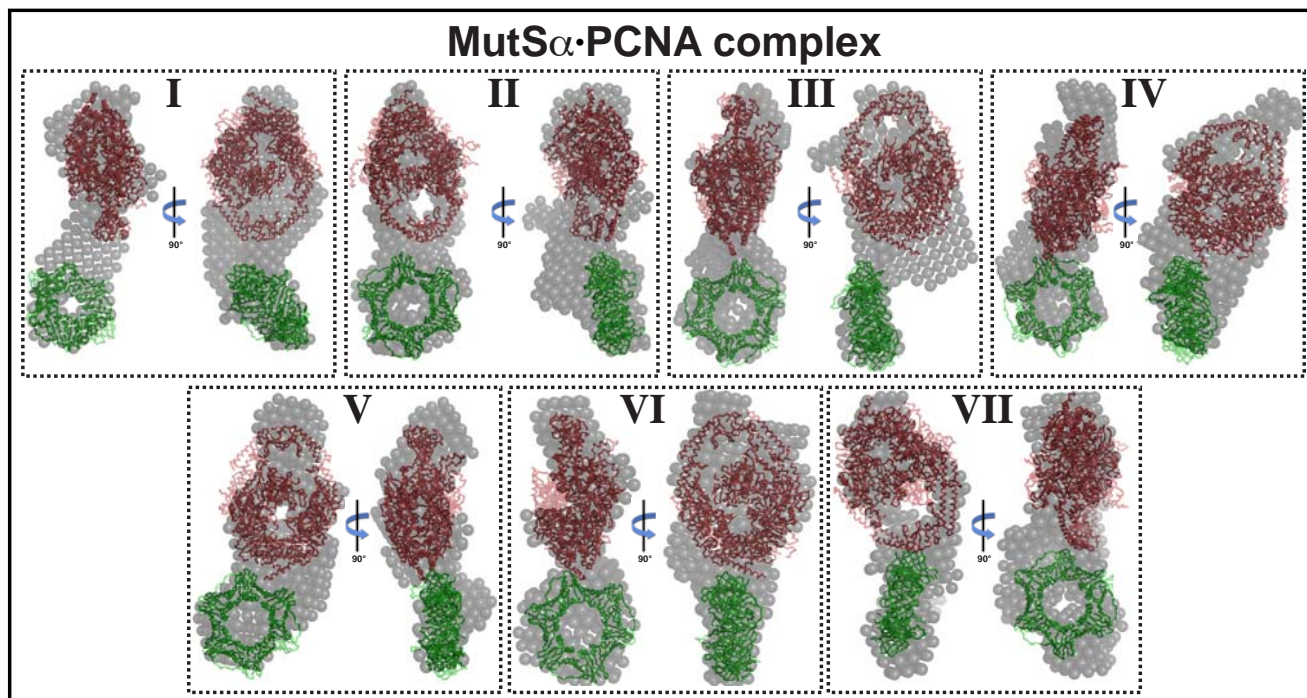
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Supplemental Fig. 2



Supplemental Fig. 3



Supplemental Fig. 4

