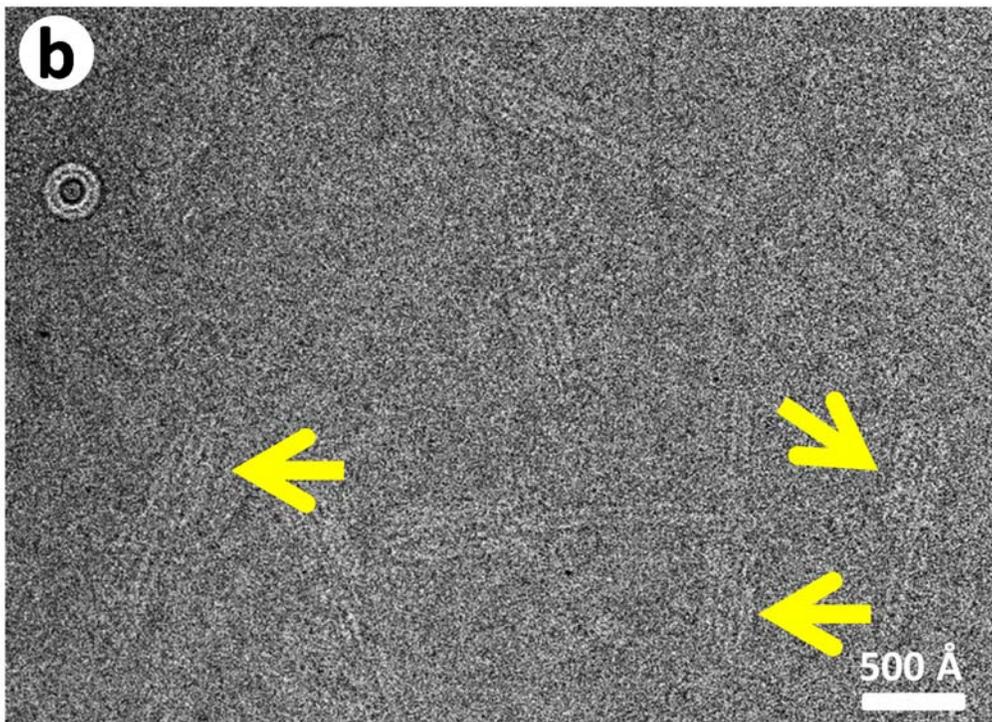
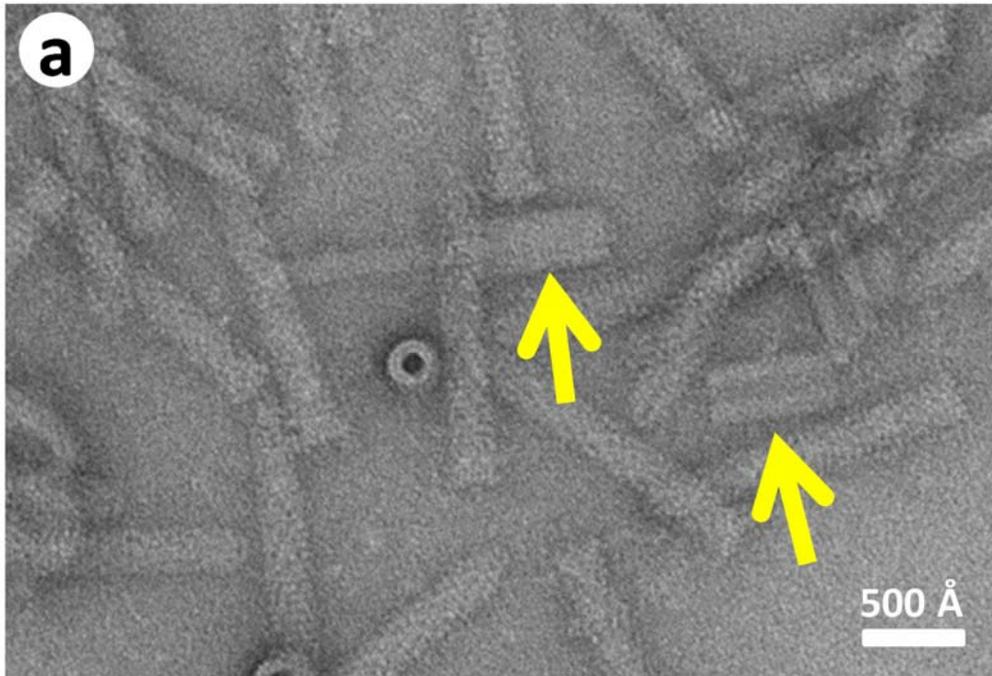


Supplementary Figure 1

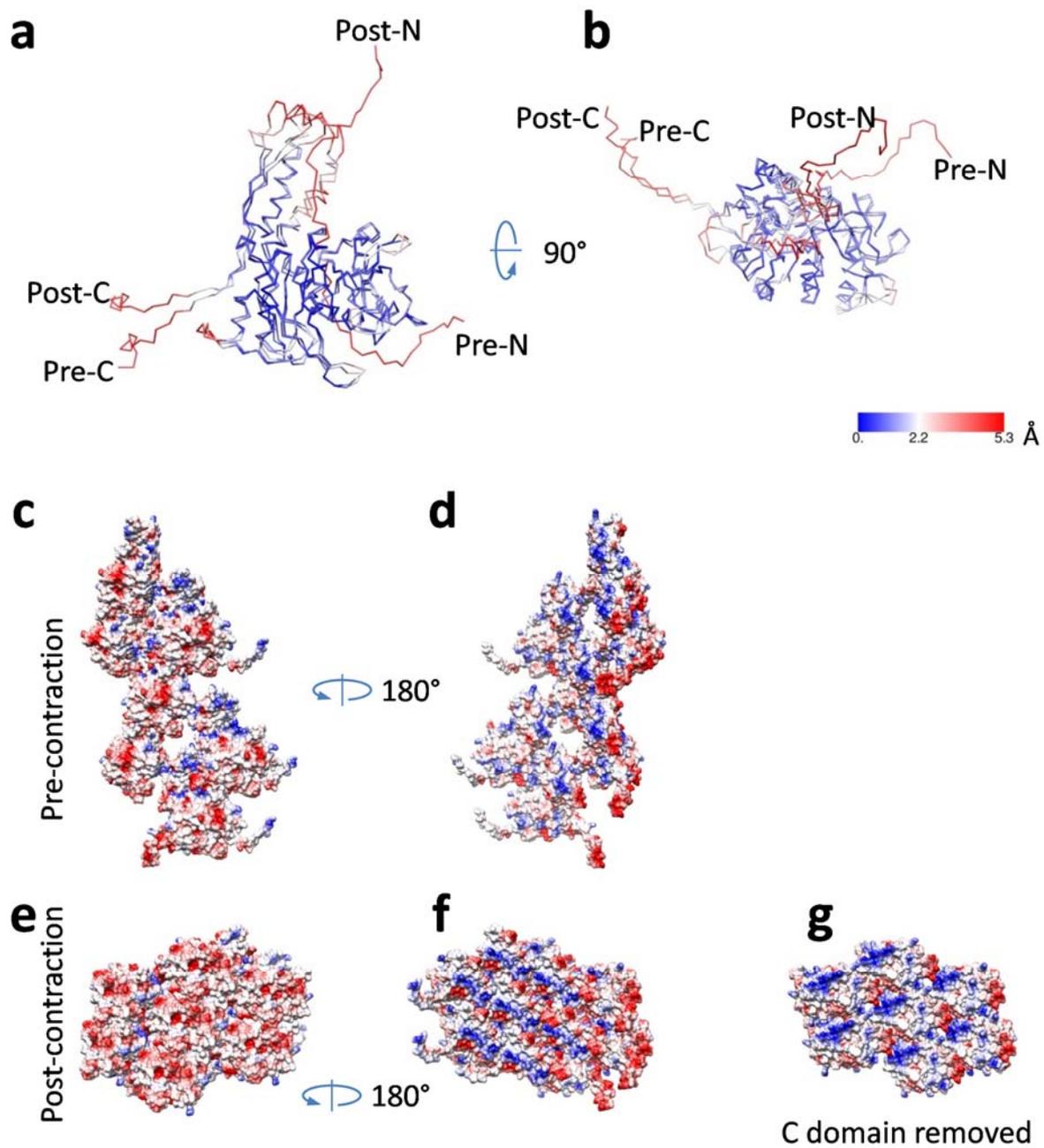
Surface charge of the top (left) and bottom (right) side of the tube hexamer.



Supplementary Figure 2

Electron microscopy images of the postcontraction pyocin R2.

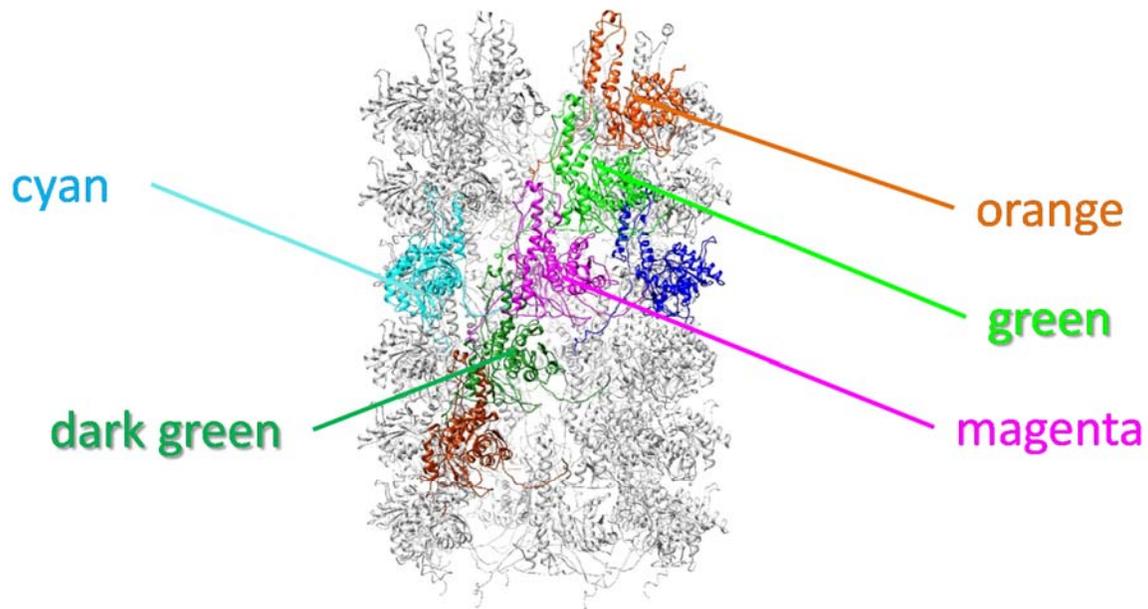
Electron microscopy images of the pyocin R2 embedded in uranyl acetate stain (a) or vitreous ice (b). Arrows point to postcontraction pyocins.



Supplementary Figure 3

Conformational change during contraction.

(a and b) Superposition of a pre- and a postcontraction sheath subunit showing extend of conformation change in different regions during contraction. (c-g) Surface charge distributions of sheath subunits in their precontraction (c and d) and postcontraction (e-g) states. For clarity, the C domain of sheath is removed in panel g.

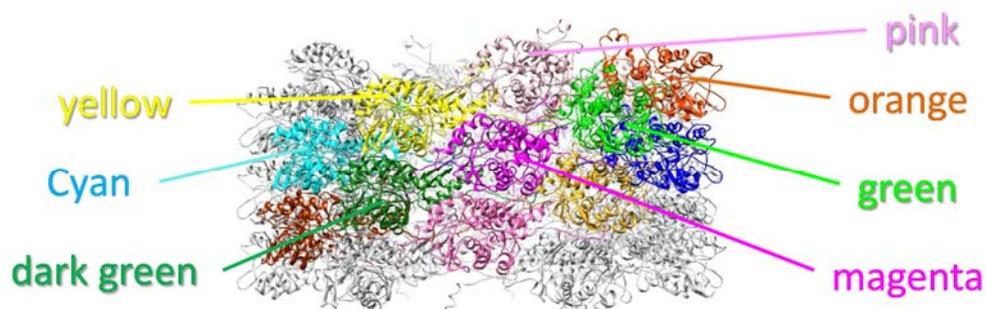


Pair of subunits	From residue(s)	To residue(s)
Magenta -> green	Glu107, Asp116	Arg234, Arg246
	Arg108, Lys149	Glu237, Glu243
	Arg151	Asp240
	Asp303	Lys224
	β -sheet augmentation Green strand Asn367-Thr375 augments Magenta sheet on strand Val353-Phe359	
Cyan -> magenta	β -sheet augmentation Cyan strand Thr8-Val12 augments Dark-green and Magenta sheet on Magenta strand Pro368-Val372	
Orange -> magenta	Leu379, Leu383	Pocket formed by magenta and green subunits

Supplementary Figure 4

Key interactions of neighboring sheath subunits in the precontraction state.

There are six neighbors for each sheath subunit. They are colored differently in the top panel; the central subunit is colored magenta. Between the magenta subunit and its six neighbors are interfaces, of which three are unique. Key residues or interactions on these interfaces are tabulated below.

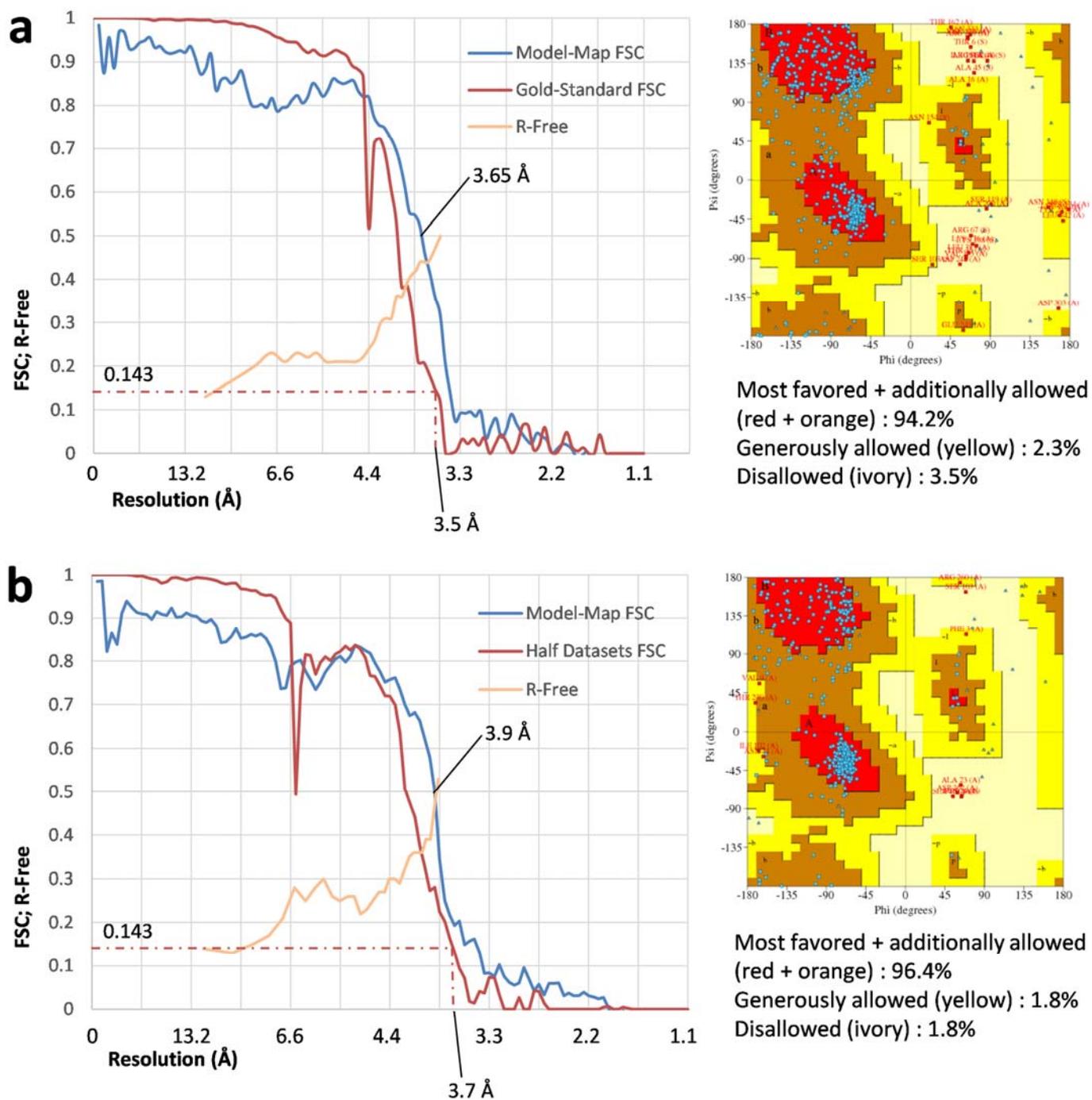


Pair of subunits	From residue(s)	To residue(s)
Magenta -> green	Lys118, Arg151	Asp240
	Lys277, Arg283	Asp376
	Lys326	Glu381
	β-sheet augmentation Green strand Asn367-Thr375 augments Magenta sheet on strand Val353-Phe359	
Cyan -> magenta	β-sheet augmentation Cyan strand Thr8-Val12 augments Dark-green and Magenta sheet on Magenta strand Pro368-Val372	
Orange -> magenta	Asp384	Lys308, Lys312
	Helix 377-383 attaches to a groove formed by magenta and green subunits	
Magenta -> pink	Asp275	Arg265
	Glu148	Arg75, Lys227
	Lys171	Asp261
Magenta -> yellow	Asp275	Arg17, Arg304
	Lys227	Asp13
	Arg246	Asp54
	Glu164	Arg120

Supplementary Figure 5

Key interactions of neighboring sheath subunits in the postcontraction state.

There are ten neighbors for each sheath subunit. They are colored differently in the top panel; the central subunit is colored magenta. Between the magenta subunit and its ten neighbors are interfaces, of which five are unique. Key residues or interactions on these interfaces are tabulated below.



Supplementary Figure 6

Resolution assessment and validation of the pre- and postcontraction structures.

(left column) Fourier shell correlation curves between maps calculated from half datasets (dark red) and between the atomic model and the map (navy blue) and R-Free factors (orange) are plotted in the same graph versus resolution, for the pre- (a) and postcontraction (b) states, respectively. (right column) Ramachandran plots for the pre- (a) and postcontraction (b) state structures. Occupancy of different areas in each plot is listed at the bottom side of it.