

Supplementary Table 1. Data collection and refinement statistics

	Mre11-DNA1 <sup>1</sup>	Mre11-DNA2 <sup>1</sup>
<b>Data collection</b>		
Wavelength (Å)	0.9795	0.9795
Space group	P2 <sub>1</sub>	P2 <sub>1</sub>
Cell dimensions a,b,c (Å)	91.5 185.6 106.2	90.5 184.0 106.6
α, β, γ (°)	90 99.9 90	90 99.5 90
Resolution <sup>2</sup> (Å)	50-3.55 (3.6-3.55)	50-3.52 (3.58-3.52)
Measured reflections	318,323	194,226
Unique reflections	41,919	42,468
Completeness (%)	100 (100)	98.8 (98.8)
Average (I/σ)	13.3 (2.3)	13 (2.5)
$R_{\text{sym}}$ <sup>3</sup>	0.166 (0.971)	0.200 (0.950)
Resolution (Å) ( $R_{\text{sym}} < 0.5$ ) <sup>4</sup>	3.82	3.83
<b>Refinement</b>		
Resolution range (Å)	42.42-3.55	47.29-3.59
No. reflections	39,539	39,755
$R_{\text{working}}$ (%) / $R_{\text{free}}$ (%) <sup>5</sup>	18.4/23.6	19.4/25.3
No. atoms (B-factors (Å <sup>2</sup> ))		
Total	16104 (144.4)	16013 (181.9)
Protein	15480 (143)	15480 (179.5)
DNA/Mg <sup>2+</sup>	592/ 12 (189.3/ 70.8)	533/ - (256.9/ -)
water	20 (66.8)	-
R.m.s. bond lengths (Å)	0.009	0.005
R.m.s. bond angles (°)	1.2	1.1
Ramachandran plot <sup>6</sup>		
Favored (%)	94.9	93.2
Allowed (%)	4.5	6.3
Disallowed (%)	0.6	0.5

<sup>1</sup>Mg<sup>2+</sup> ions are added in the crystallization buffer for the Mre11-DNA1 and -DNA2 complexes. However, we observed the clear Mg<sup>2+</sup> ion density only in the Mre11-DNA1 structure.

<sup>2</sup>Values in parentheses are for the highest shell.

<sup>3</sup> $R_{\text{sym}} = \sum_h \sum_i |I_{h,i} - \bar{I}_h| / \sum_h \sum_i I_{h,i}$ , where  $\bar{I}_h$  is the mean intensity of the  $i$  observations of symmetry related reflections of  $h$ .

<sup>4</sup>Resolution where the  $R_{\text{sym}}$  values are lower than 0.5

<sup>5</sup> $R = \frac{\sum |F_{\text{obs}} - F_{\text{calc}}|}{\sum F_{\text{obs}}}$ , where  $F_{\text{obs}} = F_{\text{pi}}$  and  $F_{\text{calc}}$  is the calculated protein structure factor from the atomic model ( $R_{\text{free}}$  was calculated with 5% of the reflections). R.m.s. deviation in bond lengths and angles are the deviations from ideal values.

<sup>6</sup>Ramachandran plot is calculated by Molprobit (Chen et al, 2010).