

## S1 Table. X-ray Data Collection and Refinement Statistics.

**CodY C. difficile** (1-156)  
PDB Code 5N0L

### Data collection

X-ray source	DLS beamline i02
Wavelength (Å)	0.97949
Collection Temperature (K)	100
Resolution range (Å)	56.19 - 1.68
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2
Unit-cell parameters (Å, °)	$a = 120.89, b = 190.39, c = 43.51$ $\alpha = \beta = \gamma = 90.0$
Matthews coefficient/solvent content (%)	2.44 / 49.6
Number of unique reflections overall/outer shell <sup>a</sup>	115,569 / 8,396
Completeness (%), overall/outer shell <sup>a</sup>	100.0 / 99.9
$I/\sigma(I)$ , overall/outer shell <sup>a</sup>	17.1 / 1.2
$R_{\text{merge}}^b$ , overall/outer shell <sup>a</sup>	0.067 / 1.814
$CC_{1/2}^h$	0.999 / 0.515

### Refinement and model statistics

$R$ -factor <sup>c</sup> ( $R$ -free <sup>d</sup> )	0.162 (0.230)
Reflections (working/free)	109,833 / 5,726
Outer shell $R$ -factor <sup>c</sup> ( $R$ -free <sup>d</sup> )	0.312 (0.375)
Outer shell reflections (working/free)	7981 / 408
Molecules/asymmetric unit	6
Number of protein non hydrogen atoms	8,141
R.m.s. deviation from target <sup>f</sup>	
Bond lengths (Å)	0.027
Bond angles (°)	2.808
Average $B$ -factor (Å <sup>2</sup> )	38.21
Ramachandran plot <sup>g</sup>	96.8/2.9/0.4

<sup>a</sup>The outer shell corresponds to 1.72 – 1.68 Å

<sup>b</sup> $R_{\text{merge}} = \frac{\sum_{hkl} \sum_i |I_i - \langle I \rangle|}{\sum_{hkl} \sum_i \langle I \rangle}$  where  $I_i$  is the intensity of the  $i$ th measurement of a reflection with indexes  $hkl$  and  $\langle I \rangle$  is the *STATISTICALLY WEIGHTED AVERAGE REFLECTION INTENSITY*.

<sup>c</sup> $R$ -factor =  $\frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$  where  $F_o$  and  $F_c$  are the observed and calculated structure factor amplitudes, respectively.

<sup>d</sup> $R$ -free is the  $R$ -factor calculated with 5 % of the reflections chosen at random and omitted from refinement.

<sup>e</sup>Outer shell for refinement corresponds to 1.680 – 1.724 Å

<sup>f</sup>Root-mean-square deviation of bond lengths and bond angles from ideal geometry.

<sup>g</sup>Percentage of residues in preferred regions/ allowed regions/ outliers.

<sup>h</sup> $CC_{1/2}$  is the correlation coefficient between two randomly selected half data sets as described in Karplus & Diederichs (2012)