

Supplementary Table 1. Data collection and refinement statistics of HEW lysozyme

Data collection statistics	
Space group	P4 ₃ 2 ₁ 2
Cell constants (Å)	<i>a</i> = <i>b</i> = 77.326, <i>c</i> = 37.193
Beamline	SPring-8 BL26B1
Detector	CCD MSC saturnA200
Exposure time (sec /frame)	10
Wavelength (Å)	0.7
Camera distance (mm)	150
Resolution (Å)	50.0 – 1.00 (1.02 - 1.00)
Oscillation angel (deg.)	1.0
σ cut-off	0.0
$R_{\text{merge}}^{\text{a, b}}$	0.072 (0.358)
No. of measurements	984,794
No. of independent reflections	61,262
Completeness (%)	93.9 (58.1)
Multiplicity	17.1 (2.7)
Mean $\langle I/\sigma(I) \rangle$	63.8 (1.4)
Refinement statistics	
Resolution (Å)	26.804 - 1.300 (1.347 - 1.300)
No. of reflections used	28,205 (2,764)
Completeness (%)	99.63 (100.0)
$R_{\text{work}}^{\text{c}}$	0.150 (0.159)
$R_{\text{free}}^{\text{c}}$	0.186 (0.197)
Number of chains (Average B factor (Å ²))	
Protein (chain A)	1 (15.18)
Water (chain S)	231 (23.78)
Na (chain NA)	1 (10.60)
Cl (chain CL)	4 (16.32)
Ethylene glycol (chain E)	1 (21.07)
R.m.s. deviations	
Bond lengths (Å)	0.015
Bond angles (°)	1.596

^a $R_{\text{merge}} = \sum_i ||I(h) - \langle I(h) \rangle| / \sum_i I(h)$, where $I(h)$ is the mean intensity after i rejections.

^b Values in parentheses are for highest resolution shells.

^c $R_{\text{work}} = \sum |F_p - F_{\text{pc}}| / \sum |F_p|$; R_{free} , the same as R_{work} but calculated on 5% data excluded from refinement