

Table S1: Details of collection data and statistics.

Protein	BambL/leX
Data collection	
Wavelength (Å)	1.140
Space group	P 2 ₁ 3
Cell dimensions a, b, c (Å)	81.4, 81.4, 81.4
Resolution (outer shell) (Å)	40.72-1.60 (1.69-1.60)
Measured/Unique reflections	21930/1180
Average multiplicity (outer shell)	6.2 (3.4)
Rmerge (outer shell)	0.04 (0.1)
Completeness (%) (outer shell)	96.2 (82.4)
Mean I/oI (outer shell)	26.6 (7.9)
Wilson B	17.4
Refinement	
Rcryst/Rfree	15.5/18.9
r.m.s.d. bonds (Å)	0.016
r.m.s.d. angles (°)	1.71
r.m.s.d. chiral (Å ³)	0.10
Protein atoms	1357
Bfac (Å ²)	14.4
Ligand atoms	156
Bfac (Å ²)	21.0
Water molecules	237
Bfac (Å ²)	27.72
PDB code	3ZW1