

SUPPORTING TABLE 1.

Data collection

Space group	C2
Unit cell dimensions (Å)	$a = 179.71; b = 41.73; c = 108.40$
Resolution range (Å)	48.8 – 1.8
Total number of reflections	291,336
Unique reflections	43,900

Model refinement

Maximum resolution (Å)	1.8
Number of reflections (free)	43860 (2.236)
$R_{\text{work}}/R_{\text{free}}^a$	20.7/23.6
No. of protein atoms	5392
No. of waters	197
Iron ion	1
Other solvent	1 (glycerol)

Root mean square deviations

Bonds (Å)	0.010
Angles (°)	1.23

^a $R_{\text{work}} = \frac{\sum |F_{\text{obs}} - |F_{\text{calc}}||}{\sum |F_{\text{obs}}|}$, where R_{free} is equivalent to R_{work} but calculated for a randomly chosen 4.82% of reflections omitted from the refinement process.