Supplementary information Table S1 Statistics of data collection and refinement

Data	PYL13-PP2CA
Integration Package	HKL2000
Space Group	P3
Unit Cell (Å)	111.38, 111.38, 70.41
Unit Cell (°)	90, 90, 120
Wavelength (Å)	1.0000
Resolution (Å)	40~2.38 (2.47~2.38)
R_{merge} (%)	6.4 (37.5)
I/sigma	23.1 (4.3)
Completeness (%)	99.9 (100.0)
Number of measured reflections	138,559
Number of unique reflections	38,995
Redundancy	3.6 (3.5)
Wilson B factor ($Å^2$)	46.3
R_{work} / R_{free} (%)	21.00/24.45
No. atoms	
Overall	6670
Protein	6351
Ion	12
Water	307
Other entities	0
Average B value ($Å^2$)	
Overall	40.68
Protein	40.445
Ion	41.12
Water	45.61
Other entities	0
R.m.s. deviations	
Bonds (Å)	0.009
Angle (°)	1.257
Ramachandran plot statistics (%)	
Most favourable	89.5
Additionally allowed	10.2
Generously allowed	0.0
Disallowed	0.3

Values in parentheses are for the highest resolution shell. $R_{merge}=\Sigma_h\Sigma_i|I_{h,i}-I_h|/\Sigma_h\Sigma_i I_{h,i}$, where I_h is the mean intensity of the i observations of symmetry related reflections of h. $R=\Sigma|F_{obs}-F_{calc}|/\Sigma F_{obs}$, where F_{calc} is the calculated protein structure factor from the atomic model (R_{free} was calculated with 5% of the reflections selected).