Supplementary information, Table S1 Data collection and refinement statistics.

Table S1. Data collection and refinement statistics.

	PXY	PXY-TDIF
Wavelength (Å)	0.979	0.979
Resolution range (Å)	40.9-3.24 (3.36-3.24)	39.9-2.77 (2.87-2.77)
Space group	P 4_12_12	P 4_12_12
Unit cell	92.8 92.8 255.3 90 90 90	93.7 93.7 228.7 90 90 90
Unique reflections	18344 (1776)	26768 (2598)
Completeness (%)	99.22 (97.96)	99.75 (99.65)
Mean I/sigma (I)	12.9 (5.2)	15.5 (5.3)
redundancy	6.2 (6.4)	5.4 (5.5)
Rsym (%)	14.8 (55.9)	14.1 (49.1)
Rwork	0.213 (0.309)	0.187 (0.246)
Rfree	0.256 (0.388)	0.242 (0.328)
Water	0	87
Protein residues	595	607
R.m.s.d (bonds)	0.013	0.011
R.m.s.d (angles)	2.07	1.30
Ramachandran favored	85%	91%
Ramachandran allowed	13.3%	9%
Ramachandran outliers	1.7%	0%
Average B-factor	75.20	47.70

Rsym = $\Sigma_h \Sigma_i |I_{h,i} - I_h| / \Sigma_h \Sigma_i I_{h,i}$, 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 $F_{obs} = F_P$, and F_{calc} is the calculated protein structure factor from the atomic model. The programs HKL2000 [36] and Phenix [39] were used for data processing and structure refinement, respectively. R.m.s.d. in bond lengths and angles are the deviations from ideal values.