

Supplementary information, Table S1. Crystallographic Data collection and Refinement

Statistics

	SeMet-AcrF3	Native-AcrF3
Data collection		
Beamline	SSRF BL-19U1	SSRF BL-19U1
Space group	<i>P6₅</i>	<i>P6₅</i>
Cell dimensions		
a, b, c (Å)	85.90, 85.90, 62.48	84.94, 84.94, 63.15
α , β , γ (°)	90.00, 90.00, 120.00	90.00, 90.00, 120.00
Resolution (Å)	50-2.0 (2.07-2.0)*	50-1.5 (1.55-1.5)*
R _{sym}	0.11 (0.49)	0.06 (0.40)
I/ σ I	30.7 (4.2)	48.8 (3.4)
Completeness (%)	100 (100)	99.9 (99.5)
Redundancy	22.0 (11.0)	15.4 (7.1)
Refinement		
Resolution (Å)		1.5
No. reflections		69325
R _{work} / R _{free}		0.166/0.187
No. atoms		
protein		2154
Solvent		392
B-factors (Å ²)		
Protein		32.88
Solvent		36.47
R.m.s. deviations		
Bond length (Å)		0.006
Bond angles (°)		0.881
Ramachandran plot		
Favored region		97.7
Allowed region		2.3
Outlier region		0

* Highest resolution shell is shown in parentheses.