

Table S3. X-ray crystallography data and statistics for the structure of OafB_{SPA}^{C-long}. Values in parenthesis correspond to the highest resolution shell unless otherwise stated.

Data collection	
Beamline	I04-1
Space group	P2 ₁ 2 ₁ 2 ₁
Cell dimensions	
a, b, c (Å)	56.74, 58.43, 90.03
α, β, γ (°)	90, 90, 90
Wavelength (Å)	0.9282
Resolution (Å)	47.39 – 1.08 (1.10 – 1.08)
No. unique reflections	126378 (6232)
Completeness (%)	100 (99.7)
Multiplicity	7.7 (6.4)
I/σ(I)	12.2 (1.2)
R _{merge} (%)	7.2 (102.5)
R _{pim} (%)	2.8 (52.9)
CC _{1/2}	0.999 (0.651)
Refinement	
Resolution	47.39 – 1.08
No. reflections (test set)	119910 (6379)
R _{work} / R _{free} (%)	13.6 / 14.9
CC _{work}	0.981
CC _{free}	0.979
No. atoms:	
Protein	2096
Water	360
Ligand	19
B factors (Å ²):	
Protein	13.49
Water	29.51
Ligand	19.55
RMSD bond lengths (Å)	0.0060
RMSD bond angles (°)	1.451
Ramachandran plot (%)	
Favoured	99
Allowed	1
Outliers	0
Data deposition	
PDB ID	6SE1