

S13 Table. X-ray diffraction data collection and refinement statistics.

	<i>PfYRS/Tyr-ML471</i>
Data collection	
Space group	C 2
Wavelength (Å)	0.9537
Number of images	3600
Oscillation range per image (°)	0.1
Detector	Eiger 16M
<i>Cell dimensions</i>	
a, b, c (Å)	138.21, 47.27, 140.512
α, β, γ (°)	90, 94.63, 90
Resolution (Å)	46.68 - 1.80 (1.82 - 1.80)
R _{sym}	0.086 (0.765)
R _{meas}	0.102 (0.899)
R _{pim}	0.054 (0.470)
CC1/2	0.998 (0.838)
I/ σ (I)	9.4 (1.2)
Total observations	567540 (31557)
Unique reflections	84432 (4481)
Completeness (%)	99.9 (100.0)
Multiplicity	6.7 (7.0)
Wilson B factor (Å ²)	32.5
Refinement	
Resolution (Å)	46.68 - 1.80 (1.82 - 1.80)
Reflections used in refinement	84394 (2835)
R _{free} reflections	4177 (136)
R _{work}	0.1830 (0.3172)
R _{free}	0.2198 (0.3517)
Protein molecules in asymmetric unit	2
Total nonhydrogen atoms	6159
Protein	5683
Ligand/ion	96
Solvent	380
Mean B factor (Å ²)	50.31

Protein	50.50
Ligand/ion	39.63
Solvent	50.14
RMS deviations	
Bond lengths (Å) (outliers > 4 σ)	0.017
Bond angles (°) (outliers > 4 σ)	1.52
Rotamer outliers (%)	1.09
Clashscore	6.33
C β outliers	0
Molprobit score	1.35
<i>Ramachandran Plot</i>	
Favoured (%)	98.55
Allowed (%)	1.45
Outliers (%)	0