

Table S1. Data collection and refinement statistics.

<i>Data collection</i>	Native	Phasing UO ₂ (C ₂ H ₃ O ₂) ₂	Native	SeMet
Number of crystals	1	1	1	1
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 4 ₁ 22	<i>P</i> 4 ₁ 22
Wavelength (Å)	0.9551	0.9551	0.9551	0.9786
Cell dimensions, <i>a</i> , <i>b</i> , <i>c</i> (Å)	63.1, 116.0, 123.0	63.2, 116.8, 123.4	77.4, 77.4, 108.6	76.1, 76.1, 110.7
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
Resolution range (Å) ^a	25-2.50(2.59-2.50)	44-3.10(3.21-3.10)	25-3.05(3.16-3.05)	40-4.20(4.35-4.20)
Unique reflections ^a	31805	17206	6699	4552
Degrees of data (°)	286	471	286	309
Completeness (%) ^a	99.1 (97.4)	99.9 (99.4)	99.3(98.0)	99.8 (100.0)
<i>R</i> _{sym} (%) ^a	6.1 (66.2)	16.5	8.4 (49.1)	8.7 (29.9)
Mn (<i>I</i> / <i>σ</i>) ^a	16.3 (2.0)	14.6 (1.9)	19.3 (2.7)	22.4 (8.4)
Redundancy ^a	7.3 (5.1)	16.3 (12.6)	13.7 (9.6)	12.8 (12.7)
Wilson plot <i>B</i> -factor (Å ²)	68	89	109	139
Phasing power (acentrics)				
Isomorphous		0.83		
Anomalous		0.18		
Figure of Merit (centrics) (to 4.02Å)		0.22 (0.37)		
Figure of Merit (acentrics) (to 4.02Å)		0.14 (0.30)		
<i>Refinement</i>				
Resolution range (Å) ^a	25-2.50(2.56-2.50)		25-3.05(3.12-3.05)	
<i>R</i> _{factor} (%) ^a	22.9 (30.2)		27.8 (34.9)	
Free <i>R</i> _{factor} (%) ^a	28.8 (40.1)		29.3 (41.5)	
Residue range built	A:15-212 B: 1-210 C:10-210 D: 8-210		14-210	
Free <i>R</i> reflections (%)	5.1		4.9	
Free <i>R</i> reflections, no. ^a	1600 (101)		316 (30)	
No. non-hydrogen protein atoms	6655		1630	
No. water molecules	70		0	
<i>Model quality</i>				
RMSD bond lengths (Å)	0.008		0.006	
RMSD bond angles (°)	1.106		0.881	
Mean <i>B</i> -factors				
Overall (Å ²)	79.3		146.5	
Protein atoms, (Å ²)	79.5		146.5	
Protein atoms NTD,(N-69) (Å ²)	58.7		132.9	
Protein atoms αE-EF linker (70-97) (Å ²)	80.0		148.5	
Protein atoms FAT,(98-C) (Å ²)	90.1		152.5	
Water (Å ²)	63.2		-	
Ramachandran plot (%)	92.5 / 7.5 / 0		90.4 / 9.5 / 0	
favored / allowed / disallowed				

^aParentheses indicate the highest-resolution shell.