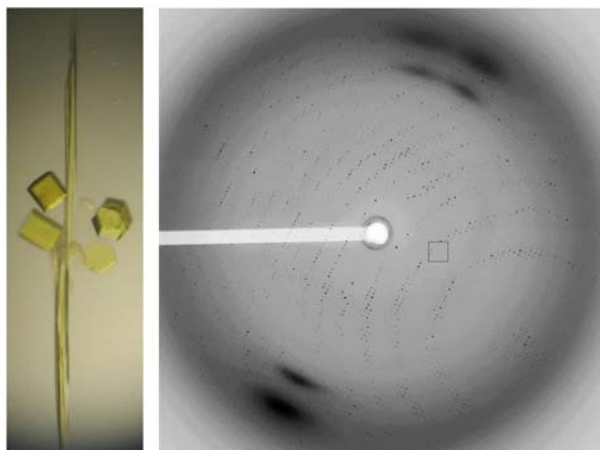


Table S1. Data collection statistics

Data collection								
	“As-purified”	Derivative (Os)			Derivative (Au)	DecylUQ	AurachinC	6.5 keV
Space group	$P2_12_12_1$	$P2_12_12_1$			$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Unit cell dimension (Å)	a = 112.85 b = 154.92 c = 178.04	a = 112.30 b = 155.86 c = 178.26			a = 112.10 b = 154.30 c = 176.70	a = 110.78 b = 154.01 c = 175.55	a = 111.18 b = 154.23 c = 176.53	a = 110.78 b = 154.01 c = 175.55
		Peak	Inflection	Remote	Peak			
Wavelength (Å)	0.91984	1.14000	1.14050	1.13010	1.03864	1.00150	1.00148	1.907445
Resolution (Å)	50.0 - 2.3 (2.4 - 2.3)	50.0 - 3.5 (3.6 - 3.5)	50.0 - 3.5 (3.6 - 3.5)	50.0 - 4.0 (4.1 - 4.0)	50.0 - 4.2 (4.3 - 4.2)	50.0 - 2.0 (2.1 - 2.0)	50.0 - 2.9 (3.0 - 2.9)	50.0 - 2.3 (2.4 - 2.3)
$R_{\text{merge}}$ (%)	8.3 (34.4)	12.3 (38.2)	12.8 (42.4)	8.2 (19.2)	6.2 (8.9)	10.5 (76.5)	8.3 (39.6)	12.4 (58.6)
$I / \sigma(I)$	14.87 (3.44)	12.69 (4.30)	12.26 (3.96)	15.77 (8.41)	15.38 (12.38)	13.17 (1.86)	16.74 (4.05)	9.97 (2.40)
Completeness (%)	97.9 (87.9)	98.9 (98.9)	98.9 (99.1)	98.7 (99.2)	99.7 (99.9)	96.2 (76.7)	98.8 (95.7)	91.1 (75.9)
Redundancy	3.47 (2.47)	3.36 (3.34)	3.37 (3.42)	3.33 (3.42)	3.83 (3.87)	4.74 (1.86)	3.72 (3.41)	2.54 (1.63)
Refinement								
Resolution (Å)	2.30					2.00	2.90	2.30
Total reflections	471,639					921,962	249,689	596,959
$R_{\text{work}} / R_{\text{free}}$ (%)	19.2 / 23.5					20.0 / 23.7	19.4 / 24.1	20.3 / 24.7
RMSD								
bond length (Å)	0.010					0.008	0.006	0.009
bond angles (°)	1.420					1.179	0.989	1.308
Number of atoms								
protein	20136					20029	20094	20029
cofactor (FAD)	318					318	318	318
detergent (DDM)	210					210	210	210
water	571					1142	194	546
ions ( $\text{SO}_4^{2-}$ )	120					120	120	120
ligand	-					138	168	138
sulfur	54					50	59	50
buffer (MES)	72					-	-	-



Five percent of the reflections were used for calculation of the  $R_{\text{free}}$ . Values in parenthesis are for the highest-resolution shell. In the *Inset* are one crystallization drop with the hexagonal and the needle crystal forms grown together and a typical diffraction pattern of the needle crystals used for solving the structure.