

**Table 3. Summary of heavy atom data sets**

Data collection								
Data set	Hg MIRAS	Pb MIRAS	Yb MIRAS	Pt MAD			I MAD	
Beam line	DESY BW7A	DESY BW7A	DESY BW7A	DESY BW7A			DESY BW7A	
Soak	10 mM HgCl <sub>2</sub>	25 mM TMLA	1 mM YbCl <sub>3</sub>	10 mM K <sub>2</sub> PtCl <sub>4</sub>			500 mM KI	
Space group	P3 <sub>1</sub> 21	P3 <sub>1</sub> 21	P3 <sub>1</sub> 21	P3 <sub>1</sub> 21			P3 <sub>1</sub> 21	
Unit cell, Å								
a = b	111.18	110.23	109.77	110.87			110.83	110.87
c	80.12	79.97	80.31	80.36			80.06	80.36
Wavelength, Å	1.072	0.8048	0.8048	1.071 (peak)	1.072 (inflection)	0.8793 (remote)	1.072 (inflection)	1.071 (peak)
Resolution (outer shell), Å	96–2.5 (2.59–2.50)	95–2.1 (2.18–2.10)	95–2.3 (2.38–2.30)	96–2.3 (2.38–2.30)	96–2.3 (2.38–2.30)	95–2.3 (2.38–2.30)	96–2.3 (2.38–2.30)	96–2.3 (2.38–2.30)
No. of observations (unique)	334.395 (20.086)	372.202 (33.338)	372.451 (25.459)	420.963 (25.718)	424.572 (25.592)	369.026 (25.548)	424.572 (25.592)	420.963 (25.718)
Completeness (outer shell), %	93.9 (96.2)	99.9 (99.9)	98.4 (98.6)	98.9 (98.7)	98.9 (98.7)	99.1 (98.1)	98.9 (98.7)	98.9 (98.7)
Data redundancy (outer shell)	4.8 (4.8)	5.9 (5.2)	3.4 (3.1)	4.3 (4.3)	4.2 (4.3)	4.3 (4.1)	4.2 (4.3)	4.3 (4.3)
I/σ <sub>1</sub> (outer shell)	18.4 (2.6)	26.2 (3.3)	15.8 (1.4)	26.5 (2.2)	26.5 (2.1)	26.9 (2.5)	26.5 (2.1)	26.5 (2.2)
R <sub>sym</sub> (outer shell), %	8.1 (53.0)	8.9 (64.5)	7.1 (72.5)	4.6 (60.9)	4.1 (60.6)	4.4 (74.1)	4.1 (60.6)	4.6 (60.9)