Table 1. Data collection and refinement statistics

	Data collection statistics:						
Dataset:	**L28B2** (native)	**L28C6** $HgCl_2$	**L28D2** K_2PtCl_4	**L88A4** $(NH_4)_2WS_4$	**L88C1** K_2OsO_4	**L88A2** EtOHg	**L88B3_2** Ta_6Br_{14}
Temperature				RT (290K)			
Spacegroup				I4			
a=b=, Å	140.7	140.9	140.8	140.2	140.6	141.0	140.9
c=, Å	97.4	97.8	97.8	97.3	98.7	96.8	96.4
Resolution, Å (final shell)	48.8 – 3.5 (3.7 – 3.5)	48.8 – 3.4 (3.6 – 3.4)	40.5 – 3.5 (3.7 – 3.5)	42.3 – 2.5 (2.7 – 2.5)	40.5 – 3.0 (3.16 – 3.0)	28.7 – 3.4 (3.58 – 3.4)	48.2 – 2.8 (2.97 – 2.8)
Reflections unique (total)	12100 (45984)	13281 (49702)	12002 (35629)	30889 (114411)	18290 (36609)	12785 (30504)	22711 (85677)
Completeness (%) overall (final shell)	100.0 (100.0)	100.0 (100.0)	98.9 (99.8)	99.0 (93.7)	95.2 (97.6)	97.4 (98.8)	99.2 (95.3)
I/σ_I overall (final shell)	2.8 (1.3)	4.1 (2.2)	3.3 (1.3)	7.9 (2.4)	2.9 (0.6)	4.5 (2.1)	2.6 (1.5)
[a]R_{merge} overall	21 %	15.7 %	18.3 %	7.7 %	19.4 %	13.7 %	15.4 %
Number of heavy atom sites	-	4	10	4	3	12	1×6
[b]Phasing power (centric/acentric)	-	0.92/1.2	0.79/1.2	0.56/0.89	0.81/1.03	1.07/1.45	1.05/1.15
[c]FOM (MIR)	0.58	-	-	-	-	-	-

	Refinement statistics:		
Dataset:	**L18B1** (native)		
Temperature	90K	Number of atoms	6445
Spacegroup	I4	Number of solvent molecules	468
a=b=, Å	138.9	Number of bounded buffer molecule atoms	66
c=, Å	94.1		
Resolution, Å (final shell)	28.0 – 1.9 (2.0 – 1.9)	Test set size	10% random
Reflections unique (total)	70374 (268268)	[d]R_{cryst} (R_{free})	0.187 (0.218)
Completeness (%) overall (final shell)	99.9 (100.0)	RMS bonds/angles	0.017 Å/1.6°
I/σ_I overall (final shell)	10.4 (2.7)	Average B-factors (Å^2)	
		main chain	25.2
		side chains	26.6
		solvent	35.5
		cofactors	56.7
[a]R_{merge} overall	4.9 %		

[a] $R_{merge} = \Sigma_h \Sigma_{i=1}^{n_h} \left| \langle I_h \rangle - I_{hi} \right| / \Sigma_h \Sigma_{i=1}^{n_h} \left| I_{hi} \right|$, where I_{hi} is an intensity value of *i*-th measurement of reflection $\boldsymbol{h}$, $\boldsymbol{h} = (h, k, l)$, sum Σ_h runs over all measured reflections, and $\langle I_h \rangle$ is an average measured intensity of the reflection $\boldsymbol{h}$. Number n_h

is a number of measurements of reflection $\boldsymbol{h}$. Data were processed with MOSFLM [Leslie 2003] and further processed SCALA [Evans 1997] and TRUNCATE [French 1978] from CCP4 [CCP4 1994] package.

[b] Phasing power = $\langle|F_{\boldsymbol{h}}^{obs}|\rangle/r.m.s.d.\,\varepsilon$, where ε is lack of closure.

[c] FOM – Figure of merit

[d] $R_{crys,free}=\Sigma_{\boldsymbol{h}}|F_{\boldsymbol{h}}^{obs}-F_{\boldsymbol{h}}^{calc}|/\Sigma_{\boldsymbol{h}}|F_{\boldsymbol{h}}^{obs}|$, where $F_{\boldsymbol{h}}^{obs}$ and $F_{\boldsymbol{h}}^{calc}$ are observed and calculated structure factors, respectively.