Table 1. Diffraction data and refinement statistics

	Native 12Y-1	LAH 12Y-1	PHR 12Y-1	Native 12Y-2
Diffraction data				
Space group	$I4_122$	$I4_122$	$I4_122$	$I2_12_12_1$
Unit cell, Å (*a*,*b*,*c*)	97.26,97.26,65.23	97.97,97.97,65.61	97.60,97.60,65.27	65.28,92.05,98.22
Resolution, Å*	69–2.8 (2.9–2.8)	20–3.0 (3.11–3.0)	20–2.5 (2.6–2.5)	67.4–2.18 (2.24–2.18)
Measured reflections	60,022	42,615	48,364	99,606
Unique reflections	3,975	3,304	5,472	15,764
Multiplicity	15.1 (4.3)	12.9 (8.3)	8.8 (5.0)	6.6 (6.3)
Completenes, %	99 (94.3)	97.2 (82.5)	96 (77)	100 (99.4)
$\langle I/\sigma(I)\rangle$	18.1 (1.8)	18.4 (1.8)	8.6 (1.5)	32.5 (4.0)
$\langle\chi^2\rangle$	1.21 (1.10)	1.74 (1.60)	1.09 (1.40)	1.19 (0.95)
$R_{merge,}$ %†	4.5	10.2	10.0	5.4
Refinement				
Resolution range, Å	6.0–2.82			18.12–2.18
R , %‡	16.6 (33.9)			17.6 (22.5)
R_{free} , %‡	25.4 (54.3)			24.7 (31.1)
RMS deviations:				
Bond length, Å	0.012			0.012
Bond angles, °	1.5			1.5
Average B values, Å^2	40.2			21.3

*Values in parentheses are for the highest shell.

†$R_{\text{merge}} = \Sigma hkl \Sigma j |Ij - \langle Ij\rangle| / \Sigma hkl \Sigma j\, |Ij|$, where *hkl* specifies unique indices, *j* indicates equivalent observations of *hkl*, and $\langle Ij\rangle$ is the mean value.

‡$R = \Sigma hkl ||Fo| - |Fc|| / \Sigma hkl\, |Fo|$, where $|Fo|$ and $|Fc|$ are the observed and calculated structure factor amplitudes, respectively.