Table 2. Statistics of BlrB structure determination

	Native	Heavy atom derivatives				
	Dark	EMP		$KAu(CN)_2$		Uranyl-acetate
PDB ID code	2byc					
Space group	$P2_12_12_1$	$P2_12_12_1$		$P2_12_12_1$		$P2_12_12_1$
Cell parameters: a,b,c, Å	36.6, 65.0, 106.9	36.7, 65.8, 107.0		36.8, 65.5, 106.6		36.7, 64.8, 106.3
Beamline	SLS XSA 06	ESRF ID 23-1		SLS XSA 06		ESRF ID 23-1
Wavelength, Å	1.071	peak 1.0052	inflection 1.00884	peak 0.90189	inflection 0.90224	1.722
Resolution of data, Å	20-1.9	10-2.3	10-2.5	10-2.8	10-2.8	10-2.3
No. of observations/ unique reflections	65,242/ 20,247	51,700/ 22,000	40,800/ 17,100	34,800/ 12,100	34,800/ 12,150	83,500/ 17,000
Completeness, total / high %*	97.1/ 98.8	99.4/ 99.8	98.7/ 98.9	99.1/ 99.4	99.1/ 99.4	99.5/ 99.7
$\langle I/\sigma(I)\rangle$, total/high %*	8.6 / 3.9	11.7 / 5.6	12.3 / 4.6	15.3 / 5.0	15.3 / 5.0	12.0 / 4.7
R_{sym},† total/high %*	9.4 / 31.9	8.8 / 23.7	10.9 / 34	5.4 / 21.3	9.7 / 31.9	6.0 / 32.6
Heavy atom conc., mM; soaking time, h		5 mM, 1h		2 mM, 12h		3mM, 1h
No. of heavy atoms		2		3		4
FOM acentric/centric	0.27/0.28					
Phasing power (full resolution range) ISO acentric/centric ANISO acentric		1.09/ 0.92 (dark) 0.93 (dark)		0.72/ 0.59 (dark) 0.68 (dark)		0.31/ 0.27 (dark) 0.25 (dark)
Resolution range, Å	15-1.9					
Included amino acids†	0-136 mol A 0-131 mol B					
No. of atoms/waters	2,316/102					
R_{work}/R_{free}, %‡	23.1/28.8					
rms deviation for bonds, Å/angles, º	0.025/2.6					

$$^{\dagger} R_{sym} = \sum_{hkl} \sum_{i} \left| I_i(hkl) - \overline{I(hkl)} \right| \Big/ \sum_{hkl} \sum_{i} I_i(hkl)$$

FOM, Figure of Merit. *, High resolution shell dark1: 1.9-2.0 Å. †, The first residue is an additional Phe, resulting from the cloning strategy. ‡, with 5% of reflections in the test set. The R_{free} values are relatively high. They do not decrease when applying different resolution or sigma cutoffs (high and/or low) or inclusion of (partial) noncrystallographic symmetry (NCS). Although we found only relatively few water molecules, there are no unexplained peaks in $F_{obs} - F_{calc}$ electron density maps. There is no indication for twinning, moreover, the R_{sym} and R_{free} values do not decrease for analyzing the data in any of the three monoclinic possibilities. The high R factors may be caused by the translational NCS (0.5, 0.5, 0.007) that relates the two monomers in the asymmetric unit (6), because it causes a departure from the assumption of randomly distributed atoms that underlies the usual interpretation of R factors (7). Refinement to 2 Å resolution results in R_{work} =21.8 and R_{free}= 27.8. Radiation damage may also affect the refinement statistics, it gets worse when including more data.