Table S1. Data collection and refinement statistics, HopBF1 structures (Related to Figure 1).

Data collection			
Crystal	HopBF1 Hg derivative (Hg peak[a])	Native HopBF1	Native HopBF1 + AMP-PNP
Space group	R32	R32	R32
Cell constants (Å)	a = 135.35, c = 124.35	a = 134.95, c = 124.49	a = 76.19, c = 351.36
Wavelength (Å)	1.00700	1.00700	0.97919
Resolution range (Å)	42.65 – 2.90 (2.95 – 2.90)	42.60 – 2.47 (2.51 – 2.47)	36.22 – 1.90 (1.93 – 1.90)
Unique reflections	9.875 (504)	15,724 (770)	31,760 (1,546)
Multiplicity	16.5 (11.1)	18.1 (16.4)	3.8 (3.7)
Data completeness (%)	100.0 (99.4)	100.0 (100.0)	99.7 (100.0)
R_{merge} (%)[b]	9.5 (131.3)	5.4 (120.8)	7.0 (121.2)
R_{pim} (%)[c]	2.4 (39.5)	1.3 (30.4)	4.0 (72.8)
I/σ(I)	27.9 (1.5)	55.8 (2.6)	11.5 (2.1)
Wilson B-value (Å^2)	43.6	28.1	20.2
Phase determination			
Anomalous scatterers	Hg, 2 major sites		
Figure of merit (42.65 – 2.90 Å)	0.19 (0.61 after density modification)		
Refinement statistics			
Crystal		Native HopBF1	Native HopBF1 + AMP-PNP
Resolution range (Å)		42.60 – 2.47 (2.55 – 2.47)	36.22 – 1.90 (1.94 – 1.90)
No. of reflections R_{work}/R_{free}		15,558/1,555 (1,126/125)	29,703/1,996 (864/63)
Data completeness (%)		99.0 (89.0)	92.9 (42.0)
Atoms (non-H protein, chain A/chain B/ nucleotide/solvent/water)		1,382/NA/NA/NA/25	1,376/1,370/62/20/232
R_{work} (%)		20.6 (26.2)	20.8 (26.7)
R_{free} (%)		22.1 (30.1)	24.0 (29.1)
R.m.s.d. bond length (Å)		0.003	0.007

R.m.s.d. bond angle (°)	0.67	0.82
Mean B-value (Å^2) (non-H protein, chain A/chain B/nucleotide/solvent/water)	47.9/NA/NA/NA/38.7	24.6/27.8/20.6/63.4/32.2
Ramachandran plot (%) (favored/additional/disallowed)[d]	95.4/4.0/0.6	98.6/1.4/0.0
Clashscore[d]	1.08	1.60
Maximum likelihood coordinate error	0.27	0.21
Missing residues	A: 0-24, 201-204.	A: 0-24, 200-204. B: 0-24, 200-204.

Data for the outermost shell are given in parentheses.

[a]Bijvoet-pairs were kept separate for data processing.

[b]$R_{merge} = 100\ \Sigma_h\Sigma_i|I_{h,i} - \langle I_h\rangle|/\Sigma_h\Sigma_i\langle I_{h,i}\rangle$, where the outer sum (h) is over the unique reflections and the inner sum (i) is over the set of independent observations of each unique reflection.

[c] $R_{pim} = 100\ \Sigma_h\Sigma_i\,[1/(n_h - 1)]^{1/2}|I_{h,i} - \langle I_h\rangle|/\Sigma_h\Sigma_i\langle I_{h,i}\rangle$, where n_h is the number of observations of reflections **h**.

[d]As defined by the validation suite *MolProbity* (Chen et al., 2010).