Table 3. Data collection and refinement statistics of the H3K4Me$_3$-bound PHD finger.

Data Collection				
	Native	**Zn MAD**		
Space group	**$P3_221$, a=b=49.18, c=52.65Å, a=β=90°, γ=120°, one molecule per A.U.**			
		peak	**inflection**	**remote**
Resolution (Å)	**2.0**	**2.0**	**2.0**	**2.2**
Wavelength (Å)	**1.54**	**1.2791**	**1.2827**	**1.2730**
Redundancy [2]	**4.4 (4.3)**	**9.8 (8.1)**	**8.1 (8.2)**	**7.8 (7.1)**
Completeness (%)	**97.0 (79.6)** [1]	**99.7 (100.0)**	**99.8 (100.0)**	**99.8 (99.7)**
Rmerge [3]	**0.039 (0.094)**	**0.080 (0.180)**	**0.097 (0.358)**	**0.111 (0.376)**
I/σ(I)	**51.1 (18.5)**	**50.4 (22.5)**	**45.1 (11.8)**	**43.0 (14.4)**
Refinement Statistics (|F|>0)				
Resolution (Å)		**30-2.0**		
$R_{working}$ (number of reflections)		**0.223**		
R_{free} [4] **(number of reflections)**		**0.231**		
Number of protein atoms		**491**		
Number of non-protein atoms		**32 water molecules and 2 zinc ions**		
R.m.s.d. from ideal bond length (Å)		**0.006**		
R.m.s.d. from ideal bond angle (o)		**1.080**		
Ramachandran statistics	**Most favored 39 residues**	**Additoinally allowed 7 residues**	**Generously allowed 1 residues**	**Disallowed** [5] **1 residue**

[1] The completeness of the 2.0-1.9Å resolution shell falls to 38% so we decided to use the 2Å data set for further refinement.

[2] Numbers in parenthesis represent values for the highest resolution bin.

[3] $R_{merge} = \Sigma| I_{obs} - I_{avg} | / \Sigma I_{avg}$.

[4] R_{free} was calculated with 10% of reflections.

[5] Residue Glu237 is clearly in a conformation which Phi/Psi values fall into the disallowed region of the Ramachandran plot.