Table 2. Summary of HDAC8 diffraction data and refinement statistics

X-ray diffraction data	
Data type	Native2
Space group	$P2_1$
Cell constants, Å	
a	51.746
b	83.532
c	94.653
β	97.485
Wavelength	0.9340
Resolution, Å*	50–2.5 (2.65–2.50)
R_{sym},† %	6.3 (44.9)
$\langle I/\sigma I \rangle$‡	9.2 (1.3)
Number of observations	184,029
Number of unique observations	27,172
Completeness, %	98.1 (98.7)
Refinement statistics	
Resolution, Å	50-2.5
R factor§	0.21
R_{free}¶	0.25
rmsd‖ bond lengths, Å	0.007
rmsd bond angles, Å	1.413
Overall B-factor, $Å^2$	42.32
φψ angle distribution**	
In core region	513 (85.5)
In allowed region	87 (14.5)
In disallowed region	0 (0)
Number of atoms	
Protein	5,478
Inhibitor	52

Ions	6
Solvent	280

*Highest resolution of the data set with the highest-resolution bin in parentheses.

†$R_{sym} = \Sigma_h\Sigma_i \mid \langle I_h \rangle - I_i(h) \mid / \Sigma_h\Sigma_i I_i(h)$, where $I_i(h)$ is the mean intensity of the N reflection.

‡Mean (I)/SD.

§R factor $= \Sigma_h |F_o - F_c| / \Sigma_h |F_o|$.

¶R_{free} is calculated from 5% of the data that were omitted during the course of the refinement.

‖ From ideal geometry.

**As defined by PROCHECK (8), the percentage distribution is given in parentheses.