Histone Deacetylase 6-Selective Inhibitors and the Influence of Capping Groups on Hydroxamate-Zinc Denticity

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SUPPORTING INFORMATION

Table S1. Data collection and refinement statistics for HDAC6-inhibitor complexes

Complex	HDAC6–**1**	HDAC6–**2**	HDAC6–**3**	HDAC6–**4**
Unit Cell				
Space group	$P2_1$	$P2_1$	$P2_1$	$P6_5$
a,b,c, (Å)	55.1, 82.5, 89.0	78.5, 95.2, 98.0	78.6, 95.5, 98.3	97.2, 97.2, 78.9
α, β, γ (°)	90.0, 98.6, 90.0	90.0, 98.9, 90.0	90.0, 98.6, 90.0	90.0, 90.0, 120.0
Data Collection				
Wavelength (Å)	0.97918	0.97918	1.18076	0.97946
Resolution (Å)	60.21–2.10	54.05–1.47	48.57–2.20	42.10–1.98
Total/unique reflections	154,035 / 45,494	899,877 / 238,509	406,680 / 21,942	282,074 / 29,613
R_{merge}[a,b]	0.236 (1.266)	0.129 (0.723)	0.228 (0.764)	0.312 (1.740)
$R_{\text{p.i.m.}}$[a,c]	0.142 (0.735)	0.077 (0.428)	0.102 (0.371)	0.106 (0.590)
$CC_{1/2}$[a,d]	0.967 (0.545)	0.989 (0.594)	0.987 (0.721)	0.990 (0.655)
$I/\sigma(I)$[a]	5.8 (3.1)	8.2 (2.8)	7.0 (2.6)	8.0 (1.9)
Redundancy[a]	3.4 (3.5)	3.8 (3.8)	5.8 (5.0)	9.5 (9.6)
Completeness (%)[a]	98.8 (98.8)	98.9 (98.7)	96.0 (92.6)	100.0 (100.0)
Refinement				
No. of reflections in refinement/test set	45551 / 4544	238405 / 23692	69,939 / 6,728	29563 / 2924
R_{work}[a,e]	0.176 (0.229)	0.148 (0.199)	0.188 (0.239)	0.168 (0.235)
R_{free}[a,e]	0.203 (0.265)	0.170 (0.229)	0.223 (0.301)	0.216 (0.273)
No. of nonhydrogen atoms				
protein	5534	11321	11109	2805
ligand	70	248	168	60
solvent	433	1861	193	222
Average *B*-factors (Å^2)				
protein	16	10	18	22
ligand	19	15	21	32
solvent	24	24	17	29
R.M.S.D. from ideal geometry				
bonds (Å)	0.002	0.009	0.002	0.004
angles (°)	0.6	1.0	0.6	0.7
Ramachandran plot (%)[f]				
favored	97.3	98.0	96.1	96.8
allowed	2.7	2.0	3.9	3.2
PDB Code	6DVL	6DVM	6DVN	6DVO

[a]Values in parentheses refer to the data from the highest resolution shell. [b]$R_{\text{merge}} = \sum_{hkl}\sum_i|I_{i,hkl} - \langle I\rangle_{hkl}|/\sum_{hkl}\sum_i I_{i,hkl}$, where $\langle I\rangle_{hkl}$ is the average intensity calculated for reflection *hkl* from replicate measurements. [c]$R_{\text{p.i.m.}} = (\sum_{hkl}(1/(N-1))^{1/2}\sum_i|I_{i,hkl} - \langle I\rangle_{hkl}|)/\sum_{hkl}\sum_i I_{i,hkl}$, where $\langle I\rangle_{hkl}$ is the average intensity calculated for reflection *hkl* from replicate measurements and N is the number of reflections [d]Pearson correlation coefficient between random half-datasets. [e]$R_{\text{work}} = \sum||F_o| - |F_c||/\sum|F_o|$ for reflections contained in the working set. $|F_o|$ and $|F_c|$ are the observed and calculated structure factor amplitudes, respectively. R_{free} is calculated using the same expression for reflections contained in the test set held aside during refinement. [f]Calculated with PROCHECK.