Inhibitor **PDB Code**	**compound 1** **9CD8**	**cyclopropyl-AMP/CoA** **8G0T**
Data Collection		
Unit-cell parameters (Å, °)	*a*=*b*=176.22 *c*=159.46	*a*=62.68 *b*=84.79 *c*=105.47 α=113.3 β=106.9 γ=91.0
Space group	$P4_12_12$	*P*1
Resolution (Å)[1]	176.22-2.40 (2.46-2.40)	91.66-2.45 (2.51-2.45)
Wavelength (Å)	0.9786	0.9786
Temperature (K)	100	100
Observed reflections	1,273,162	247,316
Unique reflections	98,167	67,989
$\langle I/\sigma(I)\rangle$[1]	13.0 (1.7)	8.1 (1.6)
Completeness (%)[1]	100 (100)	98.0 (97.7)
Multiplicity[1]	13.0 (13.5)	3.6 (2.8)
R_{merge} (%)[1, 2]	17.7 (185.4)	8.9 (83.5)
R_{meas} (%)[1, 4]	18.4 (192.7)	10.5 (97.2)
R_{pim} (%)[1, 4]	5.1 (52.3)	5.4 (49.5)
$CC_{1/2}$ [1, 5]	0.998 (0.663)	0.997 (0.789)
Refinement		
Resolution (Å) [1]	124.61-2.40	25.27-2.45
Reflections (working/test)[1]	93,205/4,864	64,534/3,312
R_{factor} / R_{free} (%)[1,3]	17.9/21.9	21.8/26.8
No. of atoms (Protein/Ligand/Water)	14,494/84/548	15,390/78/60
Model Quality		
R.m.s deviations		
Bond lengths (Å)	0.003	0.002
Bond angles (°)	0.603	0.519
Mean *B*-factor (Å^2)		
All Atoms	54.1	90.3
Protein	54.2	90.5
Ligand	70.0	75.3
Water	46.6	57.5
Coordinate error (maximum likelihood) (Å)	0.31	0.37
Ramachandran Plot		
Most favored (%)	96.5	96.4
Additionally allowed (%)	3.3	3.6

Table 1. Crystallographic Table

1) Values in parenthesis are for the highest resolution shell.
2) $R_{merge} = \Sigma_{hkl}\Sigma_i |I_i(hkl) - \langle I(hkl)\rangle| / \Sigma_{hkl}\Sigma_i I_i(hkl)$, where $I_i(hkl)$ is the intensity measured for the *i*th reflection and $\langle I(hkl)\rangle$ is the average intensity of all reflections with indices hkl.

3) $R_{factor} = \Sigma_{hkl} ||F_{obs}(hkl)| - |F_{calc}(hkl)|| / \Sigma_{hkl} |F_{obs}(hkl)|$; Rfree is calculated in an identical manner using 5% of randomly selected reflections that were not included in the refinement.

4) R_{meas} = redundancy-independent (multiplicity-weighted) R_{merge}(5, 12). R_{pim} = precision-indicating (multiplicity-weighted) R_{merge}.
5) $CC_{1/2}$ is the correlation coefficient of the mean intensities between two random half-sets of data.