Supplementary

Table S1. X-Ray Statistics.

Statistic	CA II Salicylic Acid
Wavelength (Å)	0.9795
Resolution range (Å)	35.55 - 1.36 (1.40 - 1.36)
Space group	P 1 21 1
Unit cell: a,b,c (Å)	41.3, 42.4, 72.0
α, β, ɣ (°)	90, 104.2, 90
Total reflections	145498 (7504)
Unique reflections	48888 (3558)
Multiplicity	3.0 (2.1)
Completeness (%)	93.72 (66.69)
I/I_σ	11.6 (0.8)
Wilson B-factor (Å^2)	15.85
R_{merge}[a] **(%)**	4.54 (77.60)
R_{work}[b] **(%)**	15.44 (32.61)
R_{free}[c] **(%)**	16.67 (33.08)
R_{pim}[d] **(%)**	2.97 (58.68)
Reflections used in refinement	49449 (3514)
Reflections used for R-free	2002 (138)
Number of non-hydrogen atoms	2359
macromolecules	2128
ligands	55
solvent	176
Protein residues	258
RMS(bonds) (Å)	0.012
RMS(angles) (°)	1.21
Ramachandran favored (%)	97.7
Ramachandran allowed (%)	2.3
Ramachandran outliers (%)	0.0
Rotamer outliers (%)	1.3
Average B-factor(Å^2)	22.4
macromolecules	21.5
ligands	34.6
solvent	30.7

[a] $R_{merge} = (\Sigma | I - \langle I \rangle | / \Sigma \langle I \rangle) \times 100.$

[b] $R_{work} = (\Sigma | F_o - F_c | / \Sigma | F_o |) \times 100.$

[c] R_{free} is calculated in the same way as R_{cryst} except it is for data omitted from refinement (5% of reflections for all data sets).

[d] $R_{pim} = [(\Sigma\sqrt{1/N-1})\Sigma | I - \langle I \rangle | / \Sigma \langle I \rangle] \times 100.$

Values in parentheses correspond to those of the highest-resolution shell.