Table 4. Crystallographic data collection and model refinement statistics.

	Myxothiazol*	Azoxystrobin	MOAS	Native	Stigmatellin	UHDBT1	Famoxadone	JG144[†]	*Rsbc*$_1$
Data collection									
Resolution (Å)	50-2.7	40-2.64	50-3.0	50-2.4	50-2.5	50-2.85	50-2.20	40-2.26	50-3.2
(outer shell)	(2.80-2.70)	(2.73-2.64)	(3.11-3.00)	(2.49-2.40)	(2.59-2.50)	(2.95-2.85)	(2.25-2.20)	(2.34-2.26)	(3.11-3.20)
R_{merge}[‡]	0.066 (0.433)[§]	0.073 (0.434)	0.058 (0.384)	0.058 (0.392)	0.068 (0.449)	0.072 (0.436)	0.064 (0.431)	0.064 (0.477)	0.137 (0.480)
$\langle I \rangle / \langle \sigma_I \rangle$	15.8 (1.33)	14.1 (2.15)	21.9 (2.38)	17.7 (1.76)	24.1 (1.77)	17.1 (1.14)	17.9 (5.25)	23.4 (1.11)	10.2 (2.2)
Completeness (%)	91.8 (90.7)	95.1 (85.9)	95.5 (94.7)	85.7 (77.8)	94.7 (89.4)	85.4 (20.6)	86.7 (70.5)	96.9 (87.3)	99.6 (99.4)
Ano. R_{merge}	0.060 (0.382)	0.068 (0.334)	0.049 (0.338)	0.055 (0.366)	0.062 (0.389)	0.065 (0.397)	0.060 (0.396)	0.062 (0.419)	-
Ano. completeness(%)	86.3 (79.2)	89.5 (72.7)	91.8 (85.3)	77.4 (61.5)	89.3 (78.5)	81.4 (13.0)	78.8 (56.9)	93.8 (75.7)	-
No. unique reflections	90,291	99,945	69,377	119,745	117,666	70,581	155,226	160,625	135,428
No. free reflections	2,776	2,866	2,112	3,584	3,133	2,124	2,461	3,230	2,102
Wavelength (Å)	1.0	0.92	1.736	0.97	1.0	1.2	1.0	0.97	1.0
Model refinement									
R_{work}/R_{free}	0.245/0.297	0.223/0.270	0.259/0.307	0.232/0.282	0.238/0.281	0.216/0.279	0.239/0.290	0.244/0.282	0.224/0.254
R_{work}/R_{free} (outer shell)	0.32/0.38	0.35/0.36	0.28/0.37	0.48/0.49	0.28/0.34	0.29/0.38	0.38/0.37	0.31/0.31	0.325/0.347
No. atoms	17,125	7,131	17,233	17,454	17,064	17,371	17,497	17,304	41,688
No. res. (% cmpl.)[¶]	2,081 (96.0)	2,078 (95.9)	2,104 (97.1)	2,099 (96.9)	2,101 (97.0)	2,110 (97.4)	2,111 (97.4)	2,110 (97.4)	5,178 (90.2)
No. co-factors	5	5	5	4	5	5	5	5	30
No. sol. mol.[‖]	237	243	189	454	298	322	567	271	0
r.m.s.d. bond length (Å)	0.021	0.018	0.029	0.015	0.021	0.015	0.018	0.022	0.013
r.m.s.d. bond angle (°)	2.0	1.7	2.2	1.9	2.0	2.0	1.8	2.1	1.7
DPI (Å)**	0.361	0.322	0.454	0.279	0.304	0.424	0.254	0.215	N/A

* Statistics for all data sets were computed at –1 σ cutoff for reflection intensity; space group symmetry for all crystals is $I4_122$.

[†] The chemical structure of JG144 is S-3-anilino-5-methyl-5-(4,6-difluorophenyl)-1,3-oxazolidine-2,4-dione.

[‡] R_{merge} is defined as $\Sigma|\mathbf{I}_{h,i} - \langle \mathbf{I}_h \rangle| / \Sigma \mathbf{I}_{h,i}$, where $\mathbf{I}_{h,i}$ is the intensity for **i**th observation of a reflection with Miller index **h**, and $\langle \mathbf{I}_h \rangle$ is the mean intensity for all measured $\mathbf{I}_h$s and Friedel pairs.

[§] Values in parentheses are for the highest-resolution shells.

[¶] No. of residues in the model and percentage of completeness.

[‖] No. of solvent of molecules in the model.

** Diffraction-component precision index (S9).