Protein	Ligand name	PDB ID	Ligand PDB ID	*Data Collection*													*Structure Refinement*										
				Space group	Cell dimensions						Resolution range	Unique reflections	Rsym [a] (%)	Completeness (%)	I/σI	Rcryst[b] (%)	Rfree[c] (%)	Average B all[d] (Å²)	Average B protein[d] (Å²)	Average B ligand[d] (Å²)	Average B solvent[d] (Å²)	Wilson B (Å²)	rmsd[e] bond length (Å)	rmsd angles (deg)	Coordinate error (Å)	Ramachadran favored (%)	Ramachadran allowed (%)
					a	b	c	α	β	γ																	
Wee1	MK1775	5V5Y	8X7	$P\ 2_12_12_1$	50.08	63.10	82.46	90.00	90.00	90.00	1.90-100.00 *(1.90-1.95)*	21,197 *(1,544)*	5.1 *(36.1)*	100.0 *(100.0)*	22.2 *(4.8)*	17.1	21.5	33.5	33.5	22.5	37.0	22.8	0.006	0.98	0.19	98.04	1.96
Wee1	PD166285	5VC5	96M	$P\ 2_1$	50.53	44.40	61.98	90.00	99.97	90.00	1.93-100.00 *(1.93-1.98)*	20,256 *(1,475)*	2.8 *(31.0)*	98.4 *(99.2)*	25.1 *(3.7)*	17.6	21.7	42.5	42.9	28.0	41.0	28.1	0.012	1.37	0.20	97.30	2.70
Wee1	PHA-848125	5VC6	P48	$P\ 2_1$	50.43	44.92	64.80	90.00	102.91	90.00	2.00-100.00 *(2.00-2.05)*	18,665 *(1,378)*	4.5 *(26.5)*	96.3 *(95.3)*	20.2 *(5.6)*	22.0	26.5	34.2	34.6	27.5	28.2	25.5	0.007	1.01	0.28	96.10	3.90
Wee1	Bosutinib isomer	5VC4	XZN	$P\ 2_1$	50.67	44.25	64.80	90.00	101.73	90.00	2.10-100.00 *(2.10-2.15)*	16,101 *(1,172)*	4.8 *(34.3)*	96.7 *(98.6)*	14.4 *(3.2)*	19.3	21.2	48.8	49.2	37.1	43.9	33.1	0.002	0.64	0.23	98.44	1.56
Wee1	Bosutinib	5VC3	DB8	$P\ 2_1$	50.49	45.22	60.42	90.00	102.43	90.00	1.90-20.00 *(1.90-1.95)*	20,512 *(1,502)*	5.8 *(35.3)*	96.6 *(94.8)*	12.5 *(3.8)*	21.2	25.4	45.2	45.5	41.0	40.0	29.1	0.006	0.95	0.18	98.44	1.56
Wee1	PF-03814735	5VD2	34W	$P\ 2_1$	50.52	45.71	59.44	90.00	102.52	90.00	2.05-100.00 *(2.05-2.10)*	16,847 *(1,225)*	3.5 *(26.5)*	98.8 *(99.7)*	20.2 *(4.7)*	20.3	25.5	48.2	48.5	42.8	40.3	34.1	0.003	0.56	0.20	97.64	1.97
Wee2	MK1775	5VDK	8X7	$P\ 3_2$	68.81	68.81	58.04	90.00	90.00	120.00	2.70-20.00 *(2.70-2.77)*	8,422 *(640)*	9.7 *(57.0)*	100.0 *(100.0)*	12.4 *(3.4)*	22.5	22.8	58.2	59.0	27.8	32.3	46.1	0.003	0.70	0.48	93.75	4.30
Myt1	Dasatinib	5VCV	1N1	$P\ 2_12_12_1$	56.13	68.63	75.44	90.00	90.00	90.00	1.92-20.00 *(1.92-1.97)*	22,471 *(1,609)*	5.3 *(29.6)*	98.2 *(96.8)*	28.0 *(5.1)*	15.6	19.7	26.0	26.0	17.7	27.0	18.9	0.012	1.29	0.18	97.90	2.10
Myt1	Pelitinib	5VCW	93J	$P\ 2_1$	50.51	112.90	72.71	90.00	109.27	90.00	2.25-100.00 *(2.25-2.31)*	36,183 *(9,176)*	7.6 *(30.2)*	98.9 *(99.4)*	10.3 *(3.9)*	19.6	24.6	69.7	69.8	56.7	75.5	43.2	0.010	1.24	0.29	96.82	3.18
Myt1	Saracatinib	5VCX	H8H	$P\ 2_12_12_1$	56.48	69.43	86.53	90.00	90.00	90.00	2.70-100.00 *(2.70-2.77)*	9,718 *(712)*	4.7 *(32.8)*	99.2 *(99.9)*	27.8 *(4.8)*	20.1	24.4	54.6	55.2	39.8	35.4	49.5	0.007	1.16	0.33	95.79	3.86
Myt1[f]	MK1775	5VD0	8X7	$P\ 2_12_12_1$	46.78	53.87	113.62	90.00	90.00	90.00	2.13-100.00 *(2.13-2.19)*	16,578 *(1,193)*	5.9 *(35.8)*	99.3 *(99.4)*	17.2 *(4.1)*	19.5	23.1	40.0	40.5	29.6	30.2	27.5	0.006	0.84	0.19	97.58	2.42
Myt1[f]	PHA-848125	5VD1	P48	$P\ 2_12_12_1$	46.55	55.39	113.81	90.00	90.00	90.00	1.70-100.00 *(1.70-1.74)*	32,777 *(2,369)*	6.7 *(30.7)*	98.7 *(97.7)*	14.0 *(4.3)*	14.7	19.4	25.5	25.4	17.5	27.9	16.7	0.012	1.41	0.15	97.95	1.71
Myt1[f]	Bosutinib isomer	5VCZ	XZN	$P\ 2_12_12_1$	46.63	54.97	113.53	90.00	90.00	90.00	2.00-100.00 *(2.00-2.10)*	18,757 *(2,514)*	7.3 *(27.6)*	99.8 *(100.0)*	20.7 *(7.3)*	14.8	18.1	22.6	22.3	15.0	26.9	13.5	0.016	1.61	0.;13	97.62	2.38
Myt1[f]	Bosutinib	5VCY	DB8	$P\ 2_12_12_1$	46.63	55.00	113.66	90.00	90.00	90.00	1.56-100.00 *(1.56-1.60)*	41,721 *(3,073)*	4.8 *(35.8)*	98.3 *(98.9)*	13.9 *(2.9)*	14.0	17.8	23.1	22.3	19.4	31.1	15.2	0.007	1.18	0.12	97.64	2.36
Myt1[f]	Saracatinib	5VD3	H8H	$P\ 2_12_12_1$	47.04	54.06	114.11	90.00	90.00	90.00	1.80-100.00 *(1.80-1.85)*	27,545 *(1,996)*	5.0 *(32.1)*	99.4 *(99.8)*	17.2 *(4.4)*	16.6	20.4	29.6	29.8	21.9	28.5	18.1	0.003	0.87	0.16	95.85	3.80

[a] **Rsym = 100 xΣhΣi|Ihi-Ih|/ΣhiI where h are unique reflection indices.** [b] **Rcryst = 100 xΣ|Fobs-Fmodel|/F obs where Fobs and Fmodel are observed and calculated structure factor amplitudes respectively.** [c] **Rfree is Rcryst calculated for randomly chosen unique reflections.**

[d] **Excluding hydrogen atoms** [e] **rmsd = root-mean-square deviation from ideal values, which were excluded from the refinement.** [f] **Protein treated with Lambda phosphatase prior to crystallization.**