

Protein	Ligand name	PDB ID	Ligand PDB ID	Space group	Data Collection											Structure Refinement											
					Cell dimensions						Resolution range	Unique reflections	Rsym ^a (%)	Completeness (%)	I/σI	Rcryst ^b (%)	Rfree ^c (%)	Average B all ^d (Å ²)	Average B protein ^e (Å ²)	Average B ligand ^f (Å ²)	Average B solvent ^g (Å ²)	Wilson B (Å ²)	rmsd ^h 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 ₁ 2 ₁ 2 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	X2N	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 ₁ 2 ₁ 2 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 ₁ 2 ₁ 2 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 ^l	MK1775	5VD0	8X7	P 2 ₁ 2 ₁ 2 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 ^l	PHA-848125	5VD1	P48	P 2 ₁ 2 ₁ 2 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 ^l	Bosutinib isomer	5VCZ	X2N	P 2 ₁ 2 ₁ 2 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 ^l	Bosutinib	5VCY	DB8	P 2 ₁ 2 ₁ 2 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 ^l	Saracatinib	5VD3	H8H	P 2 ₁ 2 ₁ 2 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 x Σ|I_h - I_k| / ΣI_h where h are unique reflection indices.

^b Rcryst = 100 x Σ|F_{obs} - F_{model}| / ΣF_{obs} where F_{obs} and F_{model} 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.