Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications.

Complex	**acetyl-lysine**	**DMSO**	**MPD**	**NMP**	**1-methylquinolin 2-one**	**thymine**	**thymidine**	**5-methyl uridine**	**3'-deoxy thymidine**
PDB accession code	**4QSP**	**4QSQ**	**4QSR**	**4QSS**	**4QST**	**4QSU**	**4QSV**	**4QSW**	**4QSX**
Data Collection									
Beamline	Rikagu FR-E	Rikagu FR-E	Rikagu FR-E	Rikagu FR-E	Rikagu FR-E	Rikagu FR-E	Rikagu FR-E	Rikagu FR-E	Rikagu FR-E
Wavelength (Å)	1.5418	1.5418	1.5418	1.5418	1.5418	1.5418	1.5418	1.5418	1.5418
Resolution[a] (Å)	39.87-1.60 (1.69-1.60)	19.91-1.80 (1.90-1.80)	19.26-2.00 (2.11-2.00)	19.25-2.00 (2.11-2.00)	34.51-2.05 (2.16-2.05)	34.51-1.90 (2.00-1.90)	30.27-1.90 (2.00-1.90)	34.59-1.80 (1.90-1.80)	30.65-1.93 (2.03-1.93)
Spacegroup	*P* 6_522	*P* 6_522	*P* 6_522	*P* 6_522	*P* 6_522	*P* 6_522	*P* 6_522	*P* 6_522	*P* 6_522
Cell dimensions	*a*=*b*= 79.7, *c*= 138.7 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 79.3, *c*= 138.2 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 79.6, *c*= 139.4 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 79.4, *c*=139.4 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 79.4, *c*= 138.1 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 79.1, *c*= 138.1 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 80.1, *c*=138.8 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 79.5, *c*= 138.4 Å *α*=*β*= 90˚, *γ*= 120˚	*a*=*b*= 79.2, *c*= 136.9 Å *α*=*β*= 90˚, *γ*= 120˚
No. unique reflections[a]	34,722 (4,676)	24,099 (3,405)	18,063 (2,489)	18,037 (2,516)	16,854 (2,369)	20,904 (2,976)	21,004 (2,937)	24,186 (3,381)	19,783 (2,808)
Completeness[a] (%)	99.0 (93.9)	98.5 (98.1)	98.8 (95.6)	99.1 (97.0)	99.9 (99.7)	100.0 (100.0)	98.4 (97.0)	98.3 (96.5)	100.0 (100.0)
I/σI[a]	16.4 (3.7)	9.4 (2.0)	12.5 (2.0)	15.3 (2.0)	12.0 (2.1)	12.7 (2.2)	16.9 (2.3)	16.2 (2.6)	11.2 (2.0)
R_{merge}[a]	0.073 (0.439)	0.119 (0.842)	0.134 (0.860)	0.111 (0.869)	0.127 (0.833)	0.098 (0.854)	0.086 (0.888)	0.080 (0.798)	0.102 (0.844)
Redundancy[a]	7.6 (5.8)	5.6 (5.6)	5.7 (5.5)	6.4 (5.3)	6.3 (6.3)	7.3 (7.3)	8.6 (8.7)	9.3 (9.4)	11.2 (2.0)
Refinement									
No. atoms in refinement (P/L/O)[b]	1,137/ 8/ 329	1,132/ 4/ 283	1,113/ 16/ 230	1,115/ 7/ 202	1,094/ 12/ 256	1,130/ 9/ 239	1,123/ 17/ 243	1,148/ 18/ 268	1,133/ 16/ 226
B_f (P/L/O)[b] (Å^2)	22/ 44/ 37	24/ 26/ 40	30/ 35/ 42	28/ 32/ 44	31/ 47/ 46	29/ 39/ 45	35/ 63/ 46	29/ 48/ 43	33/ 52/ 45
R_{fact}/ R_{free}	0.165/ 0.194	0.158/ 0.194	0.158/ 0.198	0.159/ 0.192	0.178/ 0.222	0.167/ 0.203	0.173/ 0.212	0.169/ 0.205	0.184/ 0.208
rms deviation bond[c] (Å)	0.016	0.016	0.016	0.016	0.016	0.015	0.014	0.015	0.015
rms deviation angle[c] (°)	1.6	1.6	1.6	1.5	1.6	1.7	1.6	1.6	1.5
Molprobity									
Ramachandran favour (%)	100	100	100	100	99.2	100	99.3	99.3	99.3
Ramachandran allowed (%)	100	100	100	100	100	100	100	100	100

[a] Values in brackets show the statistics for the highest resolution shells.
[b] P/L/O indicate protein, ligand molecules presented in the active sites, and other (water and solvent molecules), respectively.
[c] rms indicates root-mean-square.