

TMPK of E.Coli

Contacts of ligand PENTAPHOSPHATE in PDB entry 5TMP

Complex Of E. Coli Thymidylate Kinase With The Bisubstrate Inhibitor Aztp5a;
A.Lavie, N.Ostermann, R.Brundiers, R.S.Goody, J.Reinstein, M.Konrad, I.Schlichting

Residues in contact with ligand Z5A 214 in PDB entry 5TMP

Legend:

Dist - nearest distance (Å) between atoms of the ligand and the residue

Surf - contact surface area (Å²) between the ligand and the residue

HB - hydrophilic-hydrophilic contact (hydrogen bond)

Arom - aromatic-aromatic contact

Phob - hydrophobic-hydrophobic contact

DC - hydrophobic-hydrophilic contact (destabilizing contact)

+/- - indicates presence/absence of a specific contacts

* - indicates residues contacting ligand by their side chain
(including CA atoms)

Residue	Dist	Surf	Specific contacts			
			HB	Arom	Phob	DC
11A LEU	4.8	0.9	+	-	-	-
12A GLU*	3.1	44.9	+	-	-	+
13A GLY*	3.1	18.0	+	-	-	-
14A ALA	3.0	12.8	+	-	-	-
15A GLY*	2.9	56.7	+	-	-	-
16A LYS*	3.1	52.3	+	-	-	+
17A THR*	2.8	44.5	+	-	-	+
18A THR*	4.6	10.4	+	-	-	-
39A ARG*	4.6	15.4	+	-	-	+
40A GLU*	3.6	47.4	+	-	+	+
41A PRO*	3.8	8.5	-	-	+	+
51A ARG*	2.6	55.4	+	-	-	-
55A LEU*	4.0	21.6	-	-	-	+
74A PHE*	3.2	32.7	-	+	+	-
78A ARG*	2.7	35.8	+	-	-	+
99A ASP*	3.3	32.2	+	-	-	+
100A ARG*	2.8	51.3	+	-	+	+
104A SER*	3.6	24.2	+	-	-	-
105A THR*	2.8	12.2	+	-	-	-
108A TYR*	3.0	61.1	+	+	+	+
109A GLN*	2.8	37.3	+	-	-	-
149A ARG*	3.3	81.1	+	-	+	+
153A ARG*	2.5	116.9	+	-	-	+
157A ASP*	3.5	16.0	+	-	-	+
159A ILE*	3.0	43.9	+	-	-	+
160A GLU*	3.4	21.4	+	-	-	-
167A PHE*	3.4	14.3	-	-	-	-
193A LEU*	4.0	34.5	-	-	+	+