

# CMPK of E.Coli

## Contacts of ligand CYTOSINE ARABINOSE-5'- PHOSPHATE in PDB entry 1KDR

Cytidine Monophosphate Kinase From E.Coli In Complex With Ara-Cytidine Monophosphate; T.Bertrand, P.Briozzo, L.Assairi, A.Ofiteru, N.Bucurenci, H.Munier-Lehmann, B.Golinelli-Pimpaneau, O.Barzu, A.M.Gilles

**Lig.1 Residues in contact with ligand CAR5407 in PDB entry 1KDR**

Legend:

Dist - nearest distance (Å) between atoms of the ligand and the residue  
 Surf - contact surface area (Å<sup>2</sup>) 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
501 SO4	5.5	2.8	+	-	-	-
14A SER*	4.6	8.2	+	-	-	-
18A LYS*	4.8	7.3	+	-	-	-
35A ASP*	4.6	1.4	+	-	-	-
36A SER*	3.2	12.4	+	-	-	-
37A GLY*	2.9	46.8	+	-	-	+
40A TYR*	3.5	26.3	-	+	-	+
41A ARG*	2.6	57.6	+	-	-	-
92A ARG*	4.4	4.3	+	-	-	-
97A ALA*	5.1	3.4	+	-	-	+
100A ALA*	4.0	26.9	-	-	-	-
101A SER*	3.4	20.9	-	-	-	-
104A ALA*	3.7	15.3	-	-	-	-
110A ARG*	2.7	45.9	+	-	-	-
130A GLY*	3.1	13.9	-	-	-	-
131A ARG*	2.6	101.4	+	-	+	+
132A ASP*	3.3	13.9	+	-	-	-
133A MET*	4.0	2.8	-	-	-	-
181A ARG*	5.1	9.7	-	-	-	+
185A ASP*	2.3	33.5	+	-	-	-
188A ARG*	2.8	17.2	+	-	-	-

**Lig.2 Residues in contact with ligand CAR6407 in PDB entry 1KDR**

Legend:

Dist - nearest distance (Å) between atoms of the ligand and the residue  
 Surf - contact surface area (Å<sup>2</sup>) 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)

		Specific contacts					
Residue	Dist	Surf	HB	Arom	Phob	DC	
601	SO4	4.6	9.7	+	-	-	-
14B	SER*	4.2	7.1	+	-	-	-
18B	LYS*	4.5	5.0	+	-	-	-
35B	ASP*	4.5	4.3	+	-	-	-
36B	SER*	2.7	27.8	+	-	-	-
37B	GLY*	3.0	48.6	+	-	-	+
40B	TYR*	3.3	23.8	-	+	-	+
41B	ARG*	2.5	54.5	+	-	-	-
92B	ARG*	5.3	1.4	+	-	-	-
97B	ALA*	5.3	3.3	+	-	-	+
100B	ALA*	4.1	16.6	-	-	-	+
101B	SER*	3.9	20.0	-	-	-	-
104B	ALA*	3.3	21.7	-	-	-	+
110B	ARG*	2.4	46.6	+	-	-	-
129B	ASP*	4.2	10.4	+	-	-	-
130B	GLY*	3.0	22.4	-	-	-	-
131B	ARG*	2.7	97.3	+	-	+	+
132B	ASP*	3.0	15.8	+	-	-	-
133B	MET*	4.3	0.8	-	-	-	-
181B	ARG*	5.3	6.6	+	-	-	+
185B	ASP*	3.1	26.7	+	-	-	-
188B	ARG*	4.2	5.0	+	-	-	-