

GMPK of E.coli

Contacts of ligand SO4 and 5GP in PDB entry 2ANB-

(Crystal Structure Of Oligomeric E.Coli Guanylate Kinase In Complex With Gmp; G.Hible, L.Renault, F.Schaeffer, P.Christova, A.Z.Radulescu, C.Evrin, A.M.Gilles, J.Cherfils)

Ligand-Protein Contacts (LPC) are derived with the LPC software (Sobolev V., Sorokine A., Prilusky J., Abola E.E. and Edelman M. (1999) Automated analysis of interatomic contacts in proteins. *Bioinformatics*, 15, 327-332).

There are **2** ligands in PDB entry 2ANB. Click on ligand of interest for LPC analysis.

	HET ID	Chain ID	Residue N	Number of atoms	Ligand name
lig 1	SO4		302	5	SULFATE ION
lig 2	5GP		301	24	GUANOSINE-5'-MONOPHOSPHATE

Residues in contact with ligand SO4 302 in PDB entry 2ANB

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)

		Specific contacts					
Residue		Dist	Surf	HB	Arom	Phob	DC
301	5GP	4.6	6.1	+	-	-	-
11A	ALA*	4.2	1.0	-	-	-	+
12A	PRO	3.4	7.8	+	-	-	-
13A	SER*	3.6	13.7	+	-	-	-
14A	GLY	3.2	16.1	+	-	-	-
15A	ALA*	3.0	23.9	+	-	-	+
16A	GLY*	2.9	28.4	+	-	-	-
17A	LYS*	2.8	30.1	+	-	-	+
18A	SER*	2.8	38.3	+	-	-	-
19A	SER*	5.0	1.0	+	-	-	-
138A	ARG*	3.1	24.7	+	-	-	-

Residues in contact with ligand 5GP 301 in PDB entry 2ANB

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)

		Specific contacts					
Residue	Dist	Surf	HB	Arom	Phob	DC	
302	SO4	4.6	7.5	+	-	-	-
11A	ALA	3.7	18.5	+	-	-	-
13A	SER*	4.1	11.7	+	-	-	-
17A	LYS*	3.4	21.4	+	-	-	-
38A	SER*	2.5	36.7	+	-	-	-
42A	ARG*	3.2	27.5	+	-	-	-
45A	ARG*	2.8	18.5	+	-	-	-
54A	TYR*	2.7	61.1	+	-	-	-
73A	GLU*	2.8	38.2	+	-	-	+
75A	ALA*	4.0	12.9	+	-	-	+
77A	VAL*	3.2	18.6	-	-	+	+
78A	PHE*	3.8	34.0	-	-	-	-
82A	TYR*	2.9	59.3	+	+	+	+
83A	GLY	3.3	13.0	+	-	-	+
84A	THR*	3.6	0.3	+	-	-	-
102A	ASP*	3.2	34.9	+	-	-	-
103A	ILE*	3.2	32.9	-	-	+	-
104A	ASP*	2.8	48.0	+	-	-	+
107A	GLY*	3.8	5.1	+	-	-	-
138A	ARG*	4.9	1.2	+	-	-	-
149A	ARG*	2.7	27.2	+	-	-	-
156A	GLU*	4.3	6.1	+	-	-	-