

AMPK of *E. coli*

Contacts of ligands AMP and ADP in PDB entry 2ECK –

There are 4 ligands in PDB entry 2ECK.

	HET ID	Chain ID	Residue N	Number of atoms	Ligand name
lig 1	AMP	A	215	23	ADENOSINE MONOPHOSPHATE
lig 2	ADP	A	216	27	ADENOSINE-5'-DIPHOSPHATE
lig 3	AMP	B	215	23	ADENOSINE MONOPHOSPHATE
lig 4	ADP	B	216	27	ADENOSINE-5'-DIPHOSPHATE

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). On this page you will find:

Lig.1 Residues in contact with ligand AMP 215A in PDB entry 2ECK

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	
9A	PRO*	5.5	5.2	-	-	-	+
13A	LYS*	5.9	3.5	+	-	-	-
30A	SER*	5.0	4.2	+	-	-	-
31A	THR*	2.5	32.2	+	-	-	+
32A	GLY*	3.8	19.2	+	-	-	-
35A	LEU*	3.3	32.6	-	-	+	+
36A	ARG*	2.8	40.8	+	-	-	-
53A	MET*	3.7	33.2	+	-	-	+
56A	GLY	4.2	4.2	+	-	-	-
57A	LYS	2.6	29.9	+	-	-	-
58A	LEU*	3.7	26.2	-	-	+	+
59A	VAL*	3.1	49.7	+	-	-	+
64A	VAL*	3.7	23.3	-	-	+	+
84A	ASP	5.2	0.3	+	-	-	-
85A	GLY*	2.8	25.2	+	-	-	-
86A	PHE*	4.1	1.2	-	-	-	-
88A	ARG*	3.2	64.1	+	-	+	+
92A	GLN*	2.9	38.9	+	-	-	-
123A	ARG*	5.2	1.2	+	-	-	-
156A	ARG*	3.2	24.6	+	-	-	-
158A	ASP*	3.7	20.5	+	-	-	+
167A	ARG*	3.7	27.5	+	-	-	-
216A	ADP	5.1	5.9	+	-	-	-

Lig.2 Residues in contact with ligand ADP 216A in PDB entry 2ECK

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
9A PRO*	4.3	1.4	-	-	-	+
10A GLY*	2.9	42.8	+	-	-	+
11A ALA	3.3	5.1	+	-	-	-
12A GLY*	2.9	45.5	+	-	-	-
13A LYS*	2.8	48.0	+	-	-	+
14A GLY*	2.8	25.3	+	-	-	-
15A THR*	2.8	74.4	+	-	+	+
16A GLN*	5.5	2.6	+	-	-	+
84A ASP*	4.6	1.9	+	-	-	-
119A ARG*	3.2	64.2	+	-	-	+
120A ILE*	4.8	1.3	-	-	-	-
123A ARG*	3.0	69.1	+	-	-	+
132A VAL*	3.5	14.7	+	-	-	+
133A TYR*	2.8	34.1	+	-	-	-
134A HIS*	3.1	31.9	+	-	-	+
137A PHE*	3.4	35.6	-	+	+	+
138A ASN*	4.0	8.9	+	-	+	+
156A ARG*	5.5	0.2	+	-	-	-
198A GLY	4.0	8.9	+	-	-	-
199A THR	4.4	2.3	+	-	-	-
200A LYS	3.1	25.3	+	-	-	-
201A PRO*	4.7	1.6	-	-	-	+
202A VAL*	3.5	38.3	+	-	+	+
205A VAL*	4.1	8.7	-	-	-	+
215A AMP	5.1	4.9	+	-	-	-

Lig.3 Residues in contact with ligand AMP 215B in PDB entry 2ECK

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
9B PRO*	5.4	5.4	-	-	-	+
13B LYS*	5.8	4.9	+	-	-	-
30B SER*	5.0	4.0	+	-	-	-
31B THR*	2.4	32.2	+	-	-	+
32B GLY*	3.8	19.6	+	-	-	-
35B LEU*	3.3	32.4	-	-	+	+
36B ARG*	2.9	31.4	+	-	-	-
53B MET*	3.7	33.6	+	-	-	+
56B GLY	4.3	3.9	+	-	-	-
57B LYS	2.5	31.1	+	-	-	-
58B LEU*	3.7	27.7	-	-	+	+
59B VAL*	3.1	49.7	+	-	-	+
64B VAL*	3.7	24.0	-	-	+	+
84B ASP	5.3	0.3	+	-	-	-
85B GLY*	2.8	26.5	+	-	-	-
86B PHE*	4.0	1.0	-	-	-	-
88B ARG*	3.2	61.1	+	-	+	+
92B GLN*	2.8	39.7	+	-	-	-
123B ARG*	5.2	1.0	+	-	-	-
156B ARG*	3.1	35.1	+	-	-	-
158B ASP*	3.7	9.8	+	-	-	+
167B ARG*	3.7	27.8	+	-	-	-
216B ADP	5.1	6.4	+	-	-	-

Lig.4 Residues in contact with ligand ADP 216B in PDB entry 2ECK

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
9B PRO*	4.3	1.0	-	-	-	+
10B GLY*	2.8	42.4	+	-	-	+
11B ALA	3.3	4.0	+	-	-	-
12B GLY*	2.8	42.2	+	-	-	-
13B LYS*	2.7	48.3	+	-	-	+
14B GLY*	2.8	26.9	+	-	-	-
15B THR*	2.6	74.8	+	-	+	+
16B GLN*	5.5	2.2	+	-	-	+
84B ASP*	4.7	1.6	+	-	-	-
119B ARG*	3.3	59.9	+	-	-	+
120B ILE*	4.7	1.6	-	-	-	-
123B ARG*	2.9	71.7	+	-	-	+
132B VAL*	3.6	13.1	+	-	-	+
133B TYR*	2.8	36.9	+	-	-	-
134B HIS*	3.1	31.3	+	-	-	+
137B PHE*	3.3	37.9	-	+	+	+
138B ASN*	3.9	9.9	-	-	+	+
156B ARG*	5.5	0.2	+	-	-	-
198B GLY*	4.0	6.9	+	-	-	-
199B THR	4.6	2.0	+	-	-	-
200B LYS	3.1	26.1	+	-	-	-
201B PRO*	4.6	1.8	-	-	-	+
202B VAL*	3.3	37.7	+	-	+	+
205B VAL*	4.0	10.5	-	-	-	+
215B AMP	5.1	5.2	+	-	-	-