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BioInformatics Practical - 3

Summary page:

Project Summary

Target 1 MRIILLGAPGAGKGTQAQFIMEKYGIPQISTGDMLRAAVKSGSELGKQAKDIMDAGKLVTDELVIALVKERIAQEDCRNGFLLDGFPRTIPQADAMKEAGINVDYVLEFDVPDELIVDRIVGRRVHAPSGRVYHVKFNPPKVEGKDDVTG 150

Target 1 EELTTRKDDQEETVRKRLVEYHQMTAPLIGYYSKEAEAGNTKYAKVDGTKPVAEVRADLEKILG 214

Template Results

A total of 18702 templates were found to match the target sequence. This list was filtered by a heuristic down to 50. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
C4ZUS8.1	100.00	monomer	Adenylate kinase AlphaFold DB model of KAD_ECOBW (gene: adk, organism: Escherichia coli (strain K12 / MC4100 / BW2952))
3hpq.1	100.00	monomer	Adenylate kinase Crystal structure of wild-type adenylate kinase from E. coli, in complex with Ap5A
8crg.1	100.00	monomer	Adenylate kinase E. coli adenylate kinase in complex with two ADP molecules as a result of enzymatic AP4A hydrolysis
4jzk.2	100.00	monomer	Adenylate kinase Crystal Structure of Adenylate kinase of E. Coli with ADP/AMP bound
8rj4.1	100.00	monomer	Adenylate kinase E. coli adenylate kinase in complex with two ADP molecules and Mg2+ as a result of enzymatic AP4A hydrolysis

Templates (selection):

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Summary | Templates 50 | Models 4 | Project Data

Template Results

Templates | Quaternary Structure | Sequence Similarity | Alignment | More

Build Models 0

Clear Selection

Sort	Coverage	GMQE	QSQE	Identity	Method	Oligo State	Ligands
C4ZUS8.1.A Adenylate kinase *AlphaFold DB model of KAD_ECOBW (gene: adk, organism: Escherichia coli (strain K12 / MC4100 / BW2952))*		0.96	-	100.00	AlphaFold v2	monomer ✓	None
3hpq.1.A Adenylate kinase *Crystal structure of wild-type adenylate kinase from E. coli, in complex with Ap5A*		0.94	-	100.00	X-ray, 2.0Å	monomer ✓	1 x AP5
8crg.1.A Adenylate kinase *E. coli adenylate kinase in complex with two ADP molecules as a result of enzymatic AP4A hydrolysis*		0.93	-	100.00	X-ray, 1.5Å	monomer ✓	2 x ADP, 1 x MPO
4jzk.2.A Adenylate kinase *Crystal Structure of Adenylate kinase of E. Coli with ADP/AMP bound*		0.93	-	100.00	X-ray, 1.6Å	monomer ✓	1 x ADP, 1 x AMP
8rj4.1.A Adenylate kinase *E. coli adenylate kinase in complex with two ADP molecules and Mg2+ as a result of enzymatic AP4A hydrolysis*		0.93	-	100.00	X-ray, 2.1Å	monomer ✓	2 x ADP, 1 x MG

No templates selected

Final model with 3D structure:

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Model Results Order by: GMQE

1 214

Model 01

Structure Assessment

Compare

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Oligo-State: Monomer

GMQE: 0.96

Template

C4ZUS8.1.A Adenylate kinase

AlphaFold DB model of KAD_ECOBW (gene: adk, organism: Escherichia coli (strain K12 / MC4100 / BW2952))

Seq Identity 100.00%

Coverage

Model-Template Alignment