

Supporting information

Manuscript: Pharmacological targeting of AMP-activated protein kinase and opportunities for computer-aided drug design

Authors: Marie Miglianico, Gerry A.F. Nicolaes, Dietbert Neumann

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Supp. Table 1: List of all available AMPK or AMPK yeast ortholog structures.

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PDB ID	Organism	Subunit	Domain	Ligand	Method	Resolution (Å)	Deposition Year	Publication	Remark
1Z0M	Rattus norvegicus	B1	CBM	BCD	X-ray	1,49	2005	Polekhina et al. Structure, 2005	
1Z0N	Rattus norvegicus	B1	CBM	BCD	X-ray	1,49	2005	Polekhina et al. Structure, 2005	Mutation L105M
2F15	Homo sapiens	B2	CBM	BCD	X-ray	2	2005	X	
2FH9	Saccharomyces cerevisiae	Snf1 kinase (A)	KD		X-ray	2,8	2005	Nayak et al. Structure, 2006	
2H6D	Homo sapiens	A2	KD		X-ray	1,85	2005	Littler et al. Acta Cryst F, 2010	
2LTU	Homo sapiens	A2	AID		NMR	X	2006	X	
2LU3	Rattus norvegicus	B2	CBM		NMR	X	2012	X	
2LU4	Rattus norvegicus	B2	CBM		NMR	X	2012	X	
2OOX	Schizosaccharomyces pombe	SNF1-like protein kinase ssp2 (A)	B-ID		X-ray	2,6	2007	Townley & Shapiro. Science, 2007	
		SPCC1919.03c protein (B)	AG-ID						
		Hypothetical protein C1556.08c in chromosome I (G)	All	AMP					
2OOY	Schizosaccharomyces pombe	SNF1-like protein kinase ssp2 (A)	B-ID		X-ray	2,88	2007	Townley & Shapiro. Science, 2007	
		SPCC1919.03c protein (B)	AG-ID						
		Hypothetical protein C1556.08c in chromosome I (G)	All	ATP					
2QLV	Saccharomyces cerevisiae	Carbon catabolite derepressing protein kinase (SNF1, A)	B-ID		X-ray	2,6	2007	Amodeo et al. Nature, 2007	
		Protein SIP2 (B)	CBM, AG-ID						
		Nuclear protein SNF4 (G)	All						
2QR1	Schizosaccharomyces pombe	SNF1-like protein kinase ssp2 (A)	B-ID		X-ray	2,7	2007	Jin et al. Structure, 2007	
		SPCC1919.03c protein (B)	AG-ID						
		Protein C1556.08c (G)	All	ADP					
2QRC	Schizosaccharomyces pombe	SNF1-like protein kinase ssp2 (A)	B-ID		X-ray	2,7	2007	Jin et al. Structure, 2007	
		SPCC1919.03c protein (B)	AG-ID						
		Protein C1556.08c (G)	All	ADP, AMP					
2QRD	Schizosaccharomyces pombe	SNF1-like protein kinase ssp2 (A)	B-ID		X-ray	2,41	2007	Jin et al. Structure, 2007	
		SPCC1919.03c protein (B)	AG-ID						
		Protein C1556.08c (G)	All	ATP, ADP					
2QRE	Schizosaccharomyces pombe	SNF1-like protein kinase ssp2 (A)	B-ID		X-ray	3,01	2007	Jin et al. Structure, 2007	
		SPCC1919.03c protein (B)	AG-ID						
		Protein C1556.08c (G)	All	ZMP					
2UV4	Homo sapiens	G1	CBS3, CBS4	AMP	X-ray	1,33	2007	Day et al. Acta Cryst D, 2007	
2UV5	Homo sapiens	G1	CBS3, CBS4	ZMP	X-ray	1,69	2007	Day et al. Acta Cryst D, 2007	
2UV6	Homo sapiens	G1	CBS3, CBS4	AMP	X-ray	2	2007	Day et al. Acta Cryst D, 2007	
2UV7	Homo sapiens	G1	CBS3, CBS4	AMP	X-ray	2	2007	Day et al. Acta Cryst D, 2007	
2V8Q	Rattus norvegicus	A1	B-ID		X-ray	2,1	2007	Xiao et al. Nature, 2007	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	AMP					
2V92	Rattus norvegicus	A1	B-ID		X-ray	2,4	2007	Xiao et al. Nature, 2007	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	AMP, ATP					
2V9J	Rattus norvegicus	A1	B-ID		X-ray	2,53	2007	Xiao et al. Nature, 2007	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	AMP, MgATP					

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PDB ID	Organism	Subunit	Domain	Ligand	Method	Resolution (Å)	Deposition Year	Author	Remark
2Y8L	Rattus norvegicus	A1	B-ID		X-ray	2,5	2011	Xiao et al. Nature, 2011	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	ADP, AMP					
2Y8Q	Rattus norvegicus	A1	B-ID		X-ray	2,8	2011	Xiao et al. Nature, 2011	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	ADP, AMP					
2YA3	Rattus norvegicus	A1	B-ID		X-ray	2,51	2011	Xiao et al. Nature, 2011	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	Coumarin ADP					
2YZA	Homo sapiens	A2	KD		X-ray	3,02	2007	Handa et al. Acta Cryst D, 2011	Mutation T172D
3AQV	Homo sapiens	A2	KD	Compound C	X-ray	2,08	2010	Handa et al. Acta Cryst D, 2011	Mutation T172D
3DAE	Saccharomyces cerevisiae	Carbon catabolite-derepressing protein kinase (SNF1, A)	KD		X-ray	2,9	2008	Chen et al. Nature, 2009	
3H4J	Schizosaccharomyces pombe	SNF1-like protein kinase ssp2 (A)	KD-AID		X-ray	2,8	2009	Chen et al. Nature, 2009	
3MN3	Saccharomyces cerevisiae	Carbon catabolite-derepressing protein kinase (SNF1, A)	KD		X-ray	2,38	2010	Rudolph et al. Acta Cryst F, 2010	
3T4N	Saccharomyces cerevisiae	Carbon catabolite-derepressing protein kinase (SNF1, A)	B-ID		X-ray	2,3	2011	Mayer et al. Cell Metab, 2011	
		SNF1 protein kinase subunit beta-2	AG-ID						
		Nuclear protein SNF4 (G)	All	ADP					
3TDH	Saccharomyces cerevisiae	Carbon catabolite-derepressing protein kinase (SNF1, A)	B-ID		X-ray	2,3	2011	Mayer et al. Cell Metab, 2011	
		SNF1 protein kinase subunit beta-2	AG-ID						
		Nuclear protein SNF4 (G)	All	AMP					
3TE5	Saccharomyces cerevisiae	Carbon catabolite-derepressing protein kinase	B-ID		X-ray	2,5	2011	Mayer et al. Cell Metab, 2011	
		SNF1 protein kinase subunit beta-2	AG-ID						
		Nuclear protein SNF4	All	NADH					
4CFE	Homo sapiens	A2	All	991, Staurosporine	X-ray	3,02	2013	Xiao et al. Nat Comm, 2013	
		B1	CBM, AG-ID						
		G1	All	AMP					
4CFF	Homo sapiens	A2	All	A769662, Staurosporine	X-ray	3,92	2013	Xiao et al. Nat Comm, 2013	
		B1	CBM, AG-ID						
		G1	All	AMP					
4CFH	Rattus norvegicus	A1	All	Staurosporine	X-ray	3,24	2013	Xiao et al. Nature, 2011	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	AMP					
4EAG	Drosophila melanogaster	EG:132E8.2 protein (A)	B-ID		X-ray	2,7	2012	Chen et al. Nat Struct Mol Biol, 2012	
	Rattus norvegicus	B1	AG-ID						
	Rattus norvegicus	G1	All	ATP					
4EAI	Rattus norvegicus (synthetic linker)	A1	B-ID		X-ray	2,29	2012	Chen et al. Nat Struct Mol Biol, 2012	
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	AMP					

Table 1 (end): List of all available AMPK or AMPK yeast ortholog structures.

PDB ID	Organism	Subunit	Domain	Ligand	Method	Resolution (Å)	Deposition Year	Author	Remark
4EAJ	Rattus norvegicus (synthetic linker)	A1	B-ID		X-ray	2,61	2012	Chen et al. Nat Struct Mol Biol, 2012	Soaked
	Homo sapiens	B2	AG-ID						
	Rattus norvegicus	G1	All	AMP, ATP					
4EAK	Rattus norvegicus (synthetic linker)	A1	B-ID		X-ray	2,5	2012	Chen et al. Nat Struct Mol Biol, 2012	
	Rattus norvegicus	B1	AG-ID						
	Rattus norvegicus	G1	All	ATP					
4EAL	Rattus norvegicus (synthetic linker)	A1	B-ID		X-ray	2,51	2012	Chen et al. Nat Struct Mol Biol, 2012	Soaked
	Rattus norvegicus	B1	AG-ID						
	Rattus norvegicus	G1	All	AMP					
4F2L	Rattus norvegicus	A1	AID		X-ray	1,5	2012	Chen et al. Nature, 2013	
4QFG	Rattus norvegicus	A1	All	Staurosporine	X-ray	3,46	2014	Calabrese et al. Structure, 2014	
		B1	CBM, AG-ID						
		G1	All	AMP					
4QFR	Rattus norvegicus	A1	All	Cl-A769662, Staurosporine	X-ray	3,34	2014	Calabrese et al. Structure, 2014	
		B1	CBM, AG-ID						
		G1	All	AMP, ADP					
4QFS	Rattus norvegicus	A1	All	Br2-A769662, Staurosporine	X-ray	3,55	2014	Calabrese et al. Structure, 2014	
		B1	CBM, AG-ID						
		G1	All	AMP, ADP					
4RED	Homo sapiens	A1	KD-AID		X-ray	2,95	2014	Li et al. Cell Res, 2015	Mutation K43A
4RER	Homo sapiens	A1	All	Staurosporine	X-ray	4,05	2014	Li et al. Cell Res, 2015	
		B2	CBM, AG-ID	BCD					
		G1	All	AMP					
4REW	Homo sapiens	A1	All	Staurosporine	X-ray	4,58	2014	Li et al. Cell Res, 2015	
		B2	(CBM), AG-ID						
		G1	All	AMP					
4YOG	Rattus norvegicus	B2	CBM		NMR	X	2015	Mobbs et al. Biochem J, 2015	
4YEE	Rattus norvegicus	B2	CBM	GBCD	NMR	X	2015	Mobbs et al. Biochem J, 2015	
4YEF	Rattus norvegicus	B1	CBM	GBCD	NMR	X	2015	Mobbs et al. Biochem J, 2015	

In subunit, A, B and G refer to subunits α , β , and γ respectively, while the same letters in brackets refer to the corresponding mammalian ortholog subunit. In domains, the mention All means that most of the subunit structure was resolved and other abbreviations are: CBM, carbohydrate-binding module; KD, kinase domain; AID, auto-inhibitory domain; B-ID, $\alpha\beta$ -interaction domain; AG-ID, $\alpha\beta\gamma$ -interaction domain; CBS: cystathione β -synthase. In ligands, BCD and GBCD refer to β -cyclodextrin and glucosyl- β -cyclodextrin. In publication, Acta Cryst D and Acta Cryst F refer to Acta Crystallographica Section D and F respectively; Cell Metab to Cell Metabolism; Nat Comm to Nature Communications; Nat Struct Mol Biol to Nature Structural & Molecular Biology; Cell Res to Cell Research and Biochem J to Biochemical Journal.