

Experimental RNA-ligand binding free energies (kJ/mol)

PDB ID	Crystal/NMR	Binding affinity (kJ/mol)	Dissociation constant and comments	References
1F1T ¹	Crystal	-42.23	$K_D \approx 0.04\mu\text{M}$	(Baugh et al. 2000; Detering and Varani 2004; Wang et al. 2005)
1F27 ¹	Crystal	-29.8	$K_D \approx 6.0\mu\text{M}$	(Wilson et al. 1998; Detering and Varani 2004; Wang et al. 2005)
1J7T ²	Crystal	-38.47	$K_d = 0.2 \pm 0.042\mu\text{M}$	(Wilson et al. 1998; Ryu and Rando 2001)
1NTB ^{1,2}	Crystal	-34.46	$K_d \approx 1\mu\text{M}$	(Wallace and Schroeder 1998)
1YRJ ^{1,2}	Crystal	-30.91	$K_d = 2 \pm 0.20\mu\text{M} / 6.3\mu\text{M}$	(Wong et al. 1998; Griffey et al. 1999)
2F4T ^{1,2}	Crystal	-32.49	$K_d = 2.2 \pm 0.1\mu\text{M}$	(Haddad et al. 2002; Wang et al. 2005)
2FCZ ^{1,2}	Crystal	-28.62	$K_d = 10.4 \pm 1.4\mu\text{M}$	(Bernacchi et al. 2007)
2ET8 ^{1,2}	Crystal	-27.99	$K_d = 7.8\mu\text{M} / 19 \pm 1\mu\text{M}$	(Wong et al. 1998; Haddad et al. 2002)
2O3V ^{1,2}	Crystal	-30.21	$K_a = 1.8 \pm 0.1 \times 10^5 \mu\text{M}^{-1}$	(Kondo et al. 2007)
2OE8 ¹	Crystal	-36.19	$K_d = 0.5\mu\text{M}$	(Griffey et al. 1999)
1LC4 ^{1,2}	Crystal	-33.06	$K_d = 1.5\mu\text{M} / 2 \pm 0.22\mu\text{M}$	(Wong et al. 1998; Griffey et al. 1999)
1U8D ¹	Crystal	-35.24	$K_d = 0.732\mu\text{M}$	(Batey et al. 2004; Wang et al. 2005)
1YKV ¹	Crystal	-28.72	$K_d \approx 10\mu\text{M}$	(Serganov et al. 2005)
3LA5 ¹	Crystal	-34.46	$K_d = 1 \pm 0.016\mu\text{M}$	(Wang et al. 2005; Dixon et al. 2010)
3DIL	Crystal	-40.2	$K_d = 0.10 \pm 0.03\mu\text{M}$ (with K^+ and Mg^{2+})	(Serganov et al. 2008)
3Q3Z ¹	Crystal	-49.72	$K_d = 0.0022 \pm 0.0002\mu\text{M}$	(Smith et al. 2011)
2ESI	Crystal	-27.25	$K_d = 18\mu\text{M}$	(Wong et al. 1998)
2FD0 ²	Crystal	-43.04	$K_d = 0.032 \pm 0.007\mu\text{M}$	(Bernacchi et al. 2007)
3GX3	Crystal	-23.83	$K_d = 71 \pm 2\mu\text{M}$	(Montange et al. 2009)
3GX5	Crystal	-39.55	$K_d = 0.13 \pm 0.01\mu\text{M}$	(Montange et al. 2009)
3GX7	Crystal	-25.89	$K_d = 31 \pm 1\mu\text{M}$	(Montange et al. 2009)
1FMN ¹	NMR	-35.9		(Detering and Varani 2004)
2KU0 ^{1,2}	NMR	-32.08	$K_D = 2.6\mu\text{M}$	(Wang et al. 2005; Paulsen et al. 2010)
1AM0	NMR	-28.5		(Detering and Varani 2004; Morley and Afshar 2004)
1LVJ	NMR	-39.97		(Detering and Varani 2004)
1TOB ²	NMR	-52.2		(Detering and Varani 2004; Morley and Afshar 2004)
1EHT ¹	NMR	-36.5		(Detering and Varani 2004; Morley and Afshar 2004)
1BYJ ^{1,2}	NMR	-32.73	$K_d = 2.0\mu\text{M}$ (room temperature) / $0.01\mu\text{M}$ (4°C)	(Detering and Varani 2004; Morley and Afshar 2004; Wang et al. 2005)
1PBR ^{1,2}	NMR	-38.2		(Recht et al. 1996; Ryu and Rando 2001; Morley and Afshar 2004)
1EI2 ^{1,2}	NMR	-34.23		(Morley and Afshar 2004)
1KOD ^{1,2}	NMR	-23.8		(Detering and Varani 2004; Morley and Afshar 2004)
1QD3	NMR	-30.03	$K_D = 5.9 \pm 4\mu\text{M}$; $K_D = 0.92\mu\text{M}$ (U24C mutant)	(Faber et al. 2000; Wang et al. 2005)

1KOC ^{1,2}	NMR	-24.1		(Detering and Varani 2004; Morley and Afshar 2004)
1NEM ¹	NMR	-39.9		(Detering and Varani 2004; Morley and Afshar 2004)
2TOB ²	NMR	-51.2		(Detering and Varani 2004; Morley and Afshar 2004)
2KTZ ^{1,2}	NMR	-28.98	$K_d = 9\mu\text{M}$	(Wang et al. 2005; Paulsen et al. 2010)
1Q8N ¹	NMR	-35.02	$K_D = 0.8\mu\text{M}$	(Flinders et al. 2004; Wang et al. 2005)
3SD1 ³	Crystal	-27.25	$K_{D,app} = 18\pm 1\mu\text{M}$	(Trausch et al. 2011)
2YGH ³	Crystal	-37.38	$K_d = 0.31\pm 0.06\mu\text{M}$ (G2na mutation)	(Schroeder et al. 2011)
3SKI ³	Crystal	-40.20	$K_D = 0.1\pm 0.01\mu\text{M}$ (20mM Mg^{2+})	(Pikovskaya et al. 2011)
2L94 ³	NMR	-19.78	$K_{d,app} = 360\pm 26\mu\text{M}$	(Marcheschi et al. 2011)
3GER ³	Crystal	-34.75	$K_D = 0.89\pm 0.06\mu\text{M}$	(Gilbert et al. 2009)
2G5K ³	Crystal	-36.19	$K_d = 0.5\mu\text{M}$	(Wang et al. 2005)
2BEE ³	Crystal	-40.20	$K_d = 0.1\mu\text{M}$	(Francois et al. 2004)
2BEO ³	Crystal	-39.55	$K_d = 0.13\mu\text{M}$	(Francois et al. 2004)

¹ Used in training iMDLScore1 scoring function

² Used in training iMDLScore2 scoring function

³ Used as test set

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