

Supplementary Information-Conformational transitions of Adenylate Kinase: switching by cracking

Paul C. Whitford, Osamu Miyashita, Yaakov Levy & José N. Onuchic

Complete lists of contact sets and distances(Å): ($Q_{Ligand}, \sigma_{ligand}$), (Q_{open}, σ_{open})
& ($Q_{closed}, \sigma_{closed}$)

Q_{Ligand} , N=39 (Residue i, Residue j, σ_{ij})

(14,132,7.243), (15,132,6.298), (15,138,9.338), (18,130,9.135), (18,131,7.416),
(18,132,8.966), (18,133,11.333), (28,129,11.005), (28,130,10.145), (32,85,6.710),
(33,127,8.015), (33,129,8.416), (33,130,6.161), (36,156,9.418), (36,157,10.049),
(36,158,10.616), (40,127,10.107), (40,128,10.364), (53,158,6.811), (53,167,9.202),
(54,157,7.008), (54,158,5.421), (54,163,7.373), (55,163,6.302), (55,166,7.850),
(56,163,4.912), (56,166,5.498), (56,167,5.011), (56,170,8.271), (57,166,7.118),
(57,170,6.870), (58,88,8.352), (58,89,9.104), (58,170,7.247), (58,171,8.813), (58,174,8.958),
(58,175,9.837), (137,202,7.908), (138,202,7.445)

Q_{open} , N=531 (Residue i, Residue j, σ_{ij})

(1,104,6.534), (1,105,8.123), (1,213,8.857), (1,214,10.101), (1,24,6.796), (1,26,7.514),
(1,79,6.147), (1,80,4.453), (1,81,6.392), (2,100,12.824), (2,101,9.471), (2,102,7.779),
(2,103,4.883), (2,104,5.171), (2,105,6.347), (2,72,10.264), (2,77,9.202), (2,80,4.741),
(2,81,4.971), (3,103,5.883), (3,105,4.606), (3,107,7.301), (3,20,9.155), (3,213,9.553),
(3,24,10.506), (3,26,9.639), (3,81,6.329), (3,82,4.974), (3,83,6.216), (4,103,7.087),
(4,105,6.156), (4,106,4.699), (4,107,6.285), (4,182,10.445), (4,83,4.796), (4,86,6.998),
(4,87,7.996), (4,96,11.591), (5,107,5.079), (5,109,7.278), (5,13,7.429), (5,14,8.810),
(5,16,9.699), (5,17,8.801), (5,20,10.397), (5,209,11.794), (5,82,7.018), (5,83,6.223),
(5,84,5.026), (5,85,5.871), (6,106,7.263), (6,107,5.951), (6,108,4.601), (6,109,5.961),
(6,13,7.474), (6,171,10.936), (6,175,9.072), (6,178,10.056), (6,179,8.953), (6,182,11.075),
(6,193,10.549), (6,85,5.269), (6,86,7.623), (6,87,8.695), (7,108,5.704), (7,109,4.919),
(7,11,6.350), (7,13,6.022), (7,171,9.250), (7,85,7.068), (8,109,7.754), (8,111,7.680),
(8,113,8.401), (8,116,8.657), (8,12,8.133), (8,13,8.247), (8,168,6.882), (8,171,6.722),
(8,172,8.044), (9,116,8.306), (9,120,10.325), (9,13,8.795), (9,164,8.890), (9,167,7.666),
(9,168,7.135), (9,171,7.935), (10,116,5.766), (10,119,7.718), (10,120,7.384), (11,109,7.310),
(11,111,5.466), (11,116,5.959), (11,119,8.735), (12,109,8.052), (13,109,5.777),
(13,17,7.279), (13,84,8.780), (13,85,9.437), (14,18,7.893), (14,84,8.315), (15,109,10.123),
(15,19,8.278), (15,202,7.614), (16,109,9.516), (16,202,7.789), (16,205,8.023), (16,20,6.498),
(16,206,6.862), (16,209,8.659), (17,21,6.320), (17,28,7.546), (17,82,7.994), (18,22,5.915),
(19,206,7.615), (19,209,9.288), (19,210,9.753), (19,213,11.746), (19,23,5.906),
(19,24,8.544), (20,107,11.653), (20,209,8.595), (20,213,9.387), (20,24,6.118), (20,26,7.649),
(20,82,7.862), (21,25,5.072), (21,26,4.893), (21,27,5.839), (21,28,7.236), (21,82,7.561),
(23,206,10.828), (23,210,9.093), (23,214,9.371), (24,209,12.118), (24,210,10.914),
(24,213,9.765), (24,214,9.581), (25,76,8.960), (25,79,6.558), (26,76,7.253), (26,79,5.751),
(26,80,5.580), (26,81,4.856), (26,82,6.695), (27,71,11.041), (27,76,7.165), (27,77,6.713),
(27,80,7.775), (27,81,5.284), (27,82,5.948), (28,33,9.433), (28,71,11.279), (28,82,4.624),
(28,84,6.670), (29,33,6.969), (29,34,6.762), (29,68,8.647), (29,71,8.535), (29,72,8.639),
(29,77,9.462), (29,81,7.038), (29,82,5.957), (29,83,4.945), (29,84,6.182), (30,34,6.145),
(30,36,10.162), (30,83,5.903), (30,84,5.219), (31,35,5.886), (31,64,7.533), (31,68,7.941),
(31,83,8.407), (31,84,8.113), (31,85,8.239), (31,86,7.214), (31,88,10.702), (32,36,6.270),
(33,37,6.216), (34,38,6.295), (34,64,9.059), (34,67,7.156), (34,68,7.704), (34,71,7.366),
(35,39,6.632), (35,49,7.132), (35,53,9.199), (35,59,9.176), (35,64,8.058), (35,67,7.379),
(36,40,6.850), (36,53,9.584), (37,41,6.416), (37,71,9.395), (38,43,6.626), (38,46,4.016),
(38,49,7.404), (38,67,7.452), (38,70,9.280), (39,46,4.160), (39,47,5.667), (39,49,6.452),
(39,50,5.050), (39,53,9.403), (40,47,8.484), (42,47,5.562), (43,47,6.061), (43,70,9.999),
(44,48,6.452), (45,63,7.359), (45,66,7.512), (45,67,6.942), (45,70,8.751), (46,50,5.906),
(47,51,6.402), (48,52,6.655), (48,63,8.193), (49,53,6.247), (49,59,6.871), (49,63,7.417),
(49,67,9.129), (50,54,5.956), (51,55,5.903), (51,57,8.305), (52,56,6.274), (52,57,4.911),
(52,58,6.481), (52,59,6.457), (52,60,9.253), (52,63,10.156), (53,57,5.527), (53,59,7.257),
(59,63,6.447), (59,64,6.749), (60,64,6.269), (61,65,6.039), (61,89,9.802), (61,91,8.245),
(61,92,6.383), (62,66,6.313), (63,67,6.308), (64,68,6.357), (64,86,9.941), (64,88,11.497),
(64,92,8.869), (65,101,9.507), (65,69,6.200), (65,86,10.035), (65,92,7.688), (65,95,7.245),
(65,96,6.629), (65,99,8.137), (66,70,6.129), (67,71,5.781), (68,101,9.005), (68,72,5.937),
(68,81,10.866), (68,83,9.397), (68,86,9.932), (68,96,8.750), (69,101,7.593), (69,73,6.281),

(69,99,7.858), (70,74,7.206), (71,76,9.312), (71,77,8.150), (72,101,9.159), (72,77,5.492), (72,81,7.571), (72,83,9.889), (74,78,7.377), (76,80,8.376), (77,81,5.637), (81,101,11.283), (81,102,11.165), (81,103,9.081), (83,96,11.879), (86,92,8.112), (86,96,10.092), (87,178,8.397), (87,182,10.714), (87,92,5.467), (87,93,5.392), (87,96,8.309), (88,174,7.394), (88,175,6.631), (88,178,7.411), (88,92,6.628), (89,174,6.695), (89,178,5.788), (89,93,6.220), (90,177,7.061), (90,178,5.265), (90,181,6.833), (90,94,5.772), (91,95,6.293), (92,96,6.466), (93,178,7.720), (93,181,8.498), (93,182,8.675), (93,97,6.559), (94,181,9.047), (94,98,6.333), (95,99,6.137), (96,101,5.194), (96,103,9.346), (96,182,12.333), (97,101,5.330), (97,102,5.994), (97,181,11.877), (97,185,10.560), (97,190,9.830), (102,190,7.948), (103,182,10.468), (103,190,8.234), (103,191,6.140), (104,191,5.030), (104,192,5.981), (105,192,4.842), (105,194,7.614), (105,212,9.242), (105,213,8.116), (106,182,7.356), (106,191,7.443), (106,192,6.266), (106,193,4.751), (106,194,6.422), (107,194,4.997), (107,196,6.914), (107,209,9.299), (107,212,9.453), (107,213,10.031), (108,171,13.063), (108,172,12.448), (108,179,8.179), (108,193,7.838), (108,194,6.309), (108,195,4.812), (108,196,5.907), (109,196,4.850), (109,198,5.663), (109,205,9.653), (109,209,10.587), (110,195,6.571), (110,196,5.522), (110,197,5.041), (110,198,5.094), (110,199,7.490), (111,115,6.761), (111,116,6.686), (111,119,10.519), (111,198,5.174), (111,199,5.814), (112,116,6.350), (112,197,9.240), (112,199,8.147), (113,117,5.961), (113,168,7.155), (113,169,9.137), (113,172,10.020), (114,118,6.080), (114,165,8.884), (115,119,6.070), (115,199,8.533), (116,120,6.314), (116,164,8.734), (116,168,9.159), (117,121,5.886), (117,161,6.956), (117,164,6.539), (117,165,6.950), (117,168,8.964), (118,122,6.069), (118,134,9.562), (118,136,9.343), (118,137,10.148), (119,123,7.587), (119,134,7.893), (119,137,8.400), (119,198,12.726), (119,199,11.436), (120,158,8.764), (120,159,5.597), (120,164,7.829), (120,167,12.095), (121,136,10.969), (121,155,8.116), (121,159,4.778), (121,161,5.371), (121,164,7.473), (122,134,5.665), (122,135,5.863), (122,136,7.462), (123,132,6.973), (123,133,5.505), (123,134,4.190), (123,155,6.364), (123,156,8.068), (123,158,10.471), (123,159,7.088), (123,167,16.940), (124,133,5.171), (124,135,7.231), (124,140,8.985), (124,143,9.725), (124,144,7.618), (124,153,5.706), (124,154,5.041), (124,155,4.763), (125,130,6.458), (125,131,5.603), (125,132,4.365), (125,133,5.908), (125,153,5.155), (125,154,5.091), (125,155,5.891), (125,156,7.116), (125,159,10.087), (126,130,5.567), (126,131,5.133), (126,146,6.096), (126,149,9.096), (126,151,7.504), (126,152,6.924), (126,153,4.620), (127,152,8.838), (127,154,6.782), (128,151,9.503), (130,156,10.509), (131,146,7.980), (131,148,9.238), (131,149,10.722), (132,138,8.307), (132,156,9.989), (133,138,5.176), (133,139,5.472), (133,140,6.348), (133,146,8.740), (133,147,10.016), (133,148,12.291), (133,153,8.688), (134,138,4.789), (134,139,5.252), (135,139,4.643), (135,140,7.663), (135,143,7.808), (139,143,6.276), (139,147,9.743), (140,144,6.728), (140,145,6.427), (140,147,6.094), (140,153,9.224), (141,147,6.156), (142,146,7.224), (142,147,6.719), (142,150,8.028), (144,152,6.041), (144,153,5.728), (145,150,5.576), (145,151,5.489), (145,152,4.522), (145,153,5.582), (146,150,5.049), (146,151,5.095), (146,153,5.908), (155,159,6.471), (155,160,7.470), (156,160,6.942), (157,163,7.757), (158,163,6.083), (158,164,6.723), (158,167,9.520), (159,164,6.390), (160,164,6.086), (161,165,6.030), (162,166,6.199), (163,167,6.266), (164,168,6.431), (165,169,6.411), (166,170,6.106), (167,171,6.076), (168,172,6.148), (169,173,6.205), (170,174,6.365), (171,175,5.998), (171,179,11.763), (172,176,5.547), (173,177,7.934), (174,178,7.626), (175,179,6.226), (176,180,6.455), (177,181,5.893), (178,182,6.139),

(179,183,6.263), (179,193,8.701), (179,195,9.892), (180,184,6.330), (181,185,6.306),
(182,186,5.979), (182,191,7.775), (182,193,6.594), (183,187,6.104), (183,193,6.166),
(184,188,6.050), (185,190,5.365), (185,191,6.191), (186,191,4.828), (186,192,4.901),
(186,193,5.739), (194,212,7.681), (195,212,9.853), (196,205,7.332), (196,208,7.796),
(196,209,7.986), (196,212,9.566), (197,205,7.142), (197,208,9.017), (198,205,6.798),
(200,204,6.035), (200,205,5.951), (200,208,9.767), (201,205,6.192), (202,206,6.022),
(203,207,6.176), (204,208,6.188), (204,211,10.789), (205,209,6.175), (206,210,6.509),
(207,211,6.655), (208,212,6.401), (209,213,6.058), (210,214,5.310)

Q_{closed} , $N=565$ (Residue i , Residue j , σ_{ij})

(1,104,6.208), (1,105,8.171), (1,213,9.520), (1,24,8.596), (1,26,7.445), (1,79,7.071),
(1,80,4.768), (1,81,6.676), (2,100,12.411), (2,101,8.949), (2,102,7.749), (2,103,4.742),
(2,104,5.204), (2,105,6.719), (2,72,11.066), (2,77,9.281), (2,78,10.141), (2,80,4.874),
(2,81,5.106), (3,103,5.711), (3,105,4.877), (3,107,7.552), (3,20,9.630), (3,213,10.024),
(3,26,9.316), (3,81,6.640), (3,82,4.715), (3,83,6.084), (4,103,7.084), (4,105,6.357),
(4,106,4.688), (4,107,6.317), (4,182,9.891), (4,83,4.805), (4,86,7.403), (4,87,7.935),
(4,96,11.327), (5,107,5.033), (5,109,7.415), (5,13,6.297), (5,17,8.071), (5,20,10.815),
(5,82,7.611), (5,83,6.274), (5,84,5.327), (5,85,6.949), (5,86,7.967), (5,87,8.999),
(6,106,7.044), (6,107,5.936), (6,108,4.632), (6,109,6.205), (6,13,7.466), (6,171,10.605),
(6,175,8.584), (6,178,8.008), (6,179,7.727), (6,182,9.870), (6,193,10.154), (6,87,8.300),
(7,108,5.518), (7,109,4.867), (7,11,5.841), (7,13,7.057), (7,171,8.705), (7,175,8.476),
(8,109,7.672), (8,111,7.197), (8,113,7.944), (8,116,8.372), (8,13,8.919), (8,168,6.928),
(8,171,6.328), (9,116,6.997), (9,120,8.378), (9,13,8.641), (9,164,7.564), (9,167,7.018),
(9,168,6.558), (9,171,7.529), (9,88,11.152), (10,116,5.871), (10,119,6.385), (10,120,6.132),
(10,123,8.961), (11,109,5.973), (11,111,5.736), (11,116,7.394), (11,119,8.479),
(11,198,5.959), (12,109,7.240), (12,119,9.111), (12,16,6.316), (13,109,7.019), (13,17,5.997),
(13,84,6.768), (13,85,8.104), (13,88,12.990), (14,132,7.243), (14,18,6.600), (14,28,8.925),
(14,84,6.752), (15,132,6.298), (15,138,9.338), (15,19,7.265), (15,202,7.986), (16,109,9.827),
(16,202,7.981), (16,205,7.936), (16,20,6.353), (16,206,6.637), (16,209,8.533), (17,21,6.001),
(17,28,6.516), (17,82,7.355), (17,84,7.100), (18,130,9.135), (18,131,7.416), (18,132,8.966),
(18,133,11.333), (18,22,6.216), (18,28,7.471), (19,206,7.444), (19,209,9.531), (19,210,9.729),
(19,213,11.751), (19,23,5.921), (19,24,8.209), (20,107,11.855), (20,209,8.481),
(20,213,8.997), (20,24,5.580), (20,26,7.412), (20,82,8.185), (21,25,5.122), (21,26,5.067),
(21,27,5.833), (21,28,6.239), (21,82,7.625), (22,206,12.121), (23,206,10.813), (23,210,9.370),
(23,214,9.954), (24,210,10.154), (24,213,9.075), (24,214,9.163), (26,79,7.480),
(26,80,5.775), (26,81,4.959), (26,82,6.456), (27,71,10.330), (27,76,7.034), (27,77,7.015),
(27,79,9.189), (27,80,7.313), (27,81,4.877), (27,82,5.975), (28,129,11.005), (28,130,10.145),
(28,33,9.919), (28,71,10.453), (28,82,4.742), (28,84,6.775), (29,34,7.910), (29,68,7.661),
(29,71,7.509), (29,72,8.123), (29,77,9.160), (29,81,6.863), (29,82,5.985), (29,83,5.161),
(29,84,6.067), (29,86,8.457), (30,34,6.200), (30,36,10.232), (30,84,4.723), (31,35,5.951),
(31,64,7.283), (31,67,7.905), (31,68,7.463), (31,84,6.872), (31,85,5.694), (31,86,6.453),
(31,88,9.669), (32,36,6.195), (32,53,9.086), (32,84,8.350), (32,85,6.710), (32,88,10.896),
(33,127,8.015), (33,129,8.416), (33,130,6.161), (33,37,6.087), (34,38,6.159), (34,67,7.930),
(34,68,9.060), (34,71,9.525), (35,39,6.130), (35,46,5.658), (35,49,6.759), (35,53,8.975),
(35,59,9.257), (35,63,9.909), (35,64,8.383), (35,67,8.612), (36,156,9.418), (36,157,10.049),
(36,158,10.616), (36,40,6.056), (36,53,8.735), (37,41,6.078), (38,42,5.733), (38,43,4.879),
(38,45,6.973), (38,46,5.090), (38,47,5.060), (38,67,9.984), (39,46,6.317), (39,47,4.030),
(39,50,5.791), (39,53,9.966), (40,127,10.107), (40,128,10.364), (42,47,5.110), (43,47,5.490),
(44,48,7.733), (44,63,10.793), (45,63,7.527), (45,66,8.123), (45,67,7.113), (45,70,10.210),
(46,63,7.082), (46,67,7.662), (48,52,8.088), (48,63,8.925), (49,53,6.037), (49,59,6.072),
(49,63,8.824), (50,54,6.389), (51,55,6.214), (52,56,6.454), (52,57,5.324), (52,58,6.752),
(52,59,6.140), (52,60,9.152), (52,63,12.091), (53,158,6.811), (53,167,9.202), (53,57,5.624),
(53,59,7.099), (54,157,7.008), (54,158,5.421), (54,163,7.373), (55,163,6.302), (55,166,7.850),
(56,163,4.912), (56,166,5.498), (56,167,5.011), (56,170,8.271), (57,166,7.118),

(57,170,6.870), (58,170,7.247), (58,171,8.813), (58,174,8.958), (58,175,9.837),
(58,88,8.352), (58,89,9.104), (58,92,11.742), (59,63,7.155), (59,64,6.985), (59,92,11.363),
(60,64,6.599), (61,65,5.926), (61,89,7.707), (61,91,6.928), (61,92,6.137), (62,66,6.384),
(63,67,6.645), (64,68,6.377), (64,86,8.381), (64,92,8.214), (65,69,6.166), (65,86,8.660),
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(69,95,9.858), (69,98,12.026), (69,99,9.074), (70,74,7.144), (71,76,8.931), (71,77,7.711),
(72,101,9.550), (72,77,5.315), (72,78,7.700), (72,81,7.973), (72,83,9.884), (74,78,7.716),
(76,80,7.861), (77,81,5.615), (81,101,10.820), (81,103,9.194), (83,101,11.138),
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(97,185,10.696), (97,190,10.799), (102,190,7.597), (103,182,10.298), (103,190,7.998),
(103,191,6.105), (104,191,5.078), (104,192,6.131), (105,191,5.671), (105,192,4.751),
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(117,161,6.093), (117,164,6.647), (117,165,7.726), (117,168,9.604), (118,122,6.500),
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(133,138,5.566), (133,139,5.539), (133,140,6.342), (133,146,8.578), (133,147,9.891),
(133,153,8.622), (134,138,4.801), (134,139,5.100), (134,140,7.822), (135,139,4.767),
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(144,152,5.679), (144,153,5.317), (145,150,5.086), (145,151,5.137), (145,152,4.461),
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(156,160,8.411), (156,167,13.761), (158,163,5.858), (158,164,7.239), (158,167,9.379),
(159,164,6.262), (159,167,9.944), (160,164,6.203), (161,165,6.338), (162,166,6.366),
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(168,172,6.310), (169,173,6.171), (170,174,5.787), (170,175,7.273), (171,175,4.826),
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(174,178,8.109), (175,179,8.008), (176,180,8.025), (177,181,6.414), (178,182,6.032),
(179,183,5.960), (179,193,9.149), (180,184,6.081), (181,185,6.459), (182,186,6.088),
(182,191,7.866), (182,193,7.149), (183,187,6.318), (183,193,6.358), (184,188,6.390),
(185,190,5.407), (185,191,6.194), (186,191,4.880), (186,192,5.314), (186,193,5.873),
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(209,213,6.190), (210,214,5.507)