

## COMPARING GPCR PROTEINS IN BOUND AND UNBOUND STATE:

### IHQ2.PDB – BOUND STATE

nodes = 158

average degree = 7.72151898734

avg clustering coeff = 0.544386450399

edges = 610

average shortest path = 4.42562283319

### BETWEENNESS CENTRALITY =

[0, 165, 157, 304, 378, 286, 355, 280, 328, 653, 334, 114, 0, 30, 321, 11, 25, 430, 95, 61, 82, 159, 98, 46, 127, 0, 417, 31, 200, 0, 56, 247, 98, 156, 0, 187, 74, 301, 29, 217, 270, 134, 272, 142, 282, 52, 46, 90, 39, 0, 123, 43, 145, 235, 301, 192, 360, 320, 122, 242, 253, 52, 190, 80, 195, 49, 15, 8, 74, 308, 14, 15, 174, 651, 14, 15, 238, 559, 0, 0, 58, 55, 212, 140, 124, 45, 24, 37, 0, 101, 319, 144, 324, 177, 203, 49, 372, 35, 158, 337, 250, 237, 0, 295, 66, 73, 89, 157, 37, 0, 0, 121, 151, 499, 0, 290, 0, 69, 246, 0, 35, 173, 164, 296, 337, 124, 30, 212, 110, 210, 65, 148, 243, 108, 10, 65, 113, 483, 82, 0, 0, 0, 139, 543, 87, 66, 46, 223, 0, 0, 0, 127, 314, 75, 37, 207, 54, 0, 0]

### CLOSENESS CENTRALITY

[0, 0.001488095238095238, 0.001607717041800643, 0.0017064846416382253, 0.001838235294117647, 0.0019267822736030828, 0.0020242914979757085, 0.0019455252918287938, 0.00196078431372549, 0.0018450184501845018, 0.0017094017094017094, 0.0015151515151515152, 0.001375515818431912, 0.0013888888888888889, 0.0016181229773462784, 0.0013831258644536654, 0.0013966480446927375, 0.0016051364365971107, 0.0015748031496062992, 0.0013831258644536654, 0.001392757660167131, 0.0014245014245014246, 0.0014326647564469914, 0.0013315579227696406, 0.0013986013986013986,

0.0013477088948787063, 0.0014858841010401188,  
0.001272264631043257, 0.0013812154696132596,  
0.0012578616352201257, 0.0013123359580052493,  
0.001445086705202312, 0.001483679525222552,  
0.0015552099533437014, 0.0014947683109118087,  
0.0016233766233766235, 0.001644736842105263,  
0.0017513134851138354, 0.0016051364365971107,  
0.0017006802721088435, 0.0017035775127768314,  
0.001584786053882726, 0.0016611295681063123,  
0.0014947683109118087, 0.0014903129657228018,  
0.0012547051442910915, 0.0012531328320802004,  
0.0012062726176115801, 0.00125, 0.0011123470522803114,  
0.0013245033112582781, 0.0014184397163120568,  
0.0015723270440251573, 0.0017211703958691911,  
0.0018450184501845018, 0.001869158878504673,  
0.0019569471624266144, 0.0019047619047619048,  
0.0018315018315018315, 0.0017482517482517483,  
0.001652892561983471, 0.0015360983102918587,  
0.0014771048744460858, 0.0013422818791946308,  
0.0013440860215053765, 0.0012690355329949238,  
0.001218026796589525, 0.0011947431302270011,  
0.001256281407035176, 0.001394700139470014,  
0.0013717421124828531, 0.0013736263736263737,  
0.0014367816091954023, 0.0016638935108153079,  
0.0014285714285714286, 0.0014265335235378032,  
0.001483679525222552, 0.0017035775127768314,  
0.001447178002894356, 0.0014124293785310734,  
0.0015267175572519084, 0.001466275659824047,  
0.001524390243902439, 0.0013550135501355014,  
0.001256281407035176, 0.0011507479861910242,  
0.0010799136069114472, 0.0011273957158962795,  
0.001122334455667789, 0.0012165450121654502,  
0.0013351134846461949, 0.0014204545454545455,  
0.0016181229773462784, 0.001610305958132045,  
0.0017953321364452424, 0.0018115942028985507,  
0.0019646365422396855, 0.0018281535648994515,  
0.0018587360594795538, 0.0018018018018018018,  
0.0017094017094017094, 0.0016155088852988692,  
0.0015151515151515152, 0.0014925373134328358,

0.001366120218579235, 0.0013386880856760374,  
0.0012970168612191958, 0.0012953367875647669,  
0.0011507479861910242, 0.0010822510822510823,  
0.0010559662090813093, 0.0012610340479192938,  
0.0013513513513513514, 0.0015455950540958269,  
0.0015082956259426848, 0.0016260162601626016,  
0.0014184397163120568, 0.0014534883720930232,  
0.0015873015873015873, 0.0014084507042253522,  
0.0013850415512465374, 0.001597444089456869,  
0.001584786053882726, 0.0017421602787456446, 0.0017825311942959,  
0.0016806722689075631, 0.0016313213703099511,  
0.0017730496453900709, 0.0016666666666666668,  
0.0015723270440251573, 0.0015290519877675841,  
0.0015698587127158557, 0.0014367816091954023,  
0.001392757660167131, 0.0012515644555694619,  
0.0013054830287206266, 0.001256281407035176,  
0.0013605442176870747, 0.001288659793814433,  
0.001141552511415525, 0.0011534025374855825,  
0.0012315270935960591, 0.0012437810945273632,  
0.001402524544179523, 0.0012239902080783353,  
0.0011806375442739079, 0.001182033096926714,  
0.0012674271229404308, 0.0011325028312570782,  
0.0011013215859030838, 0.001184834123222749,  
0.0012254901960784314, 0.0013679890560875513,  
0.0012919896640826874, 0.0012919896640826874,  
0.0014641288433382138, 0.0014245014245014246,  
0.0014144271570014145, 0.0015128593040847202]

PDB – 1IM6.PDB – UNBOUND STATE

nodes = 158

average degree = 7.50632911392

avg clustering coeff = 0.554656770796

edges = 593

average shortest path = 4.54906071112

BETWEENNESS CENTRALITY =

[0, 100, 207, 248, 381, 305, 343, 308, 231, 596, 328, 158, 0, 32, 416, 11, 36, 13, 383, 58, 125, 52, 130, 41, 265, 0, 496, 48, 68, 0, 49, 340, 49, 160, 0, 173, 65, 299, 129, 121, 274, 198, 127, 150, 179, 111, 6, 4, 2, 131, 86, 262, 110, 326, 340, 218, 347, 390, 117, 266, 251, 37, 157, 42, 96, 18, 374, 32, 86, 175, 69, 28, 91, 479, 50, 15, 230, 496, 113, 0, 55, 139, 399, 264, 0, 0, 0, 33, 0, 4, 299, 0, 46, 466, 146, 48, 340, 38, 129, 334, 99, 486, 39, 169, 77, 93, 98, 0, 76, 0, 0, 240, 153, 475, 44, 285, 0, 63, 238, 0, 38, 171, 258, 267, 381, 83, 25, 217, 141, 44, 101, 110, 264, 142, 100, 262, 319, 45, 395, 0, 0, 3, 187, 42, 227, 90, 61, 0, 0, 99, 240, 83, 232, 84, 20, 257, 10, 0, 0]

CLOSENESS CENTRALITY =

[0, 0.001430615164520744, 0.0015748031496062992, 0.0016806722689075631, 0.0018148820326678765, 0.0018832391713747645, 0.001976284584980237, 0.0019011406844106464, 0.0018867924528301887, 0.0018148820326678765, 0.0015723270440251573, 0.0015360983102918587, 0.0013404825737265416, 0.0013422818791946308, 0.001557632398753894, 0.0013054830287206266, 0.0013386880856760374, 0.0013422818791946308, 0.0015267175572519084, 0.001314060446780552, 0.0013477088948787063, 0.0013477088948787063, 0.0014285714285714286, 0.0013333333333333333, 0.001402524544179523, 0.0013333333333333333, 0.0014903129657228018, 0.0012738853503184713, 0.0013531799729364006, 0.0012484394506866417, 0.0013003901170351106, 0.0014577259475218659, 0.0014814814814814814, 0.0015552099533437014, 0.001483679525222552, 0.001597444089456869, 0.001610305958132045, 0.0017271157167530224, 0.0016286644951140066, 0.0016778523489932886, 0.0016638935108153079, 0.0015432098765432098, 0.001524390243902439, 0.001392757660167131, 0.001287001287001287, 0.0011587485515643105, 0.0010787486515641855, 0.0010121457489878543, 0.0010438413361169101, 0.001160092807424594, 0.0012376237623762376]

0.001402524544179523, 0.0015105740181268882,  
0.0016806722689075631, 0.0017889087656529517,  
0.0018115942028985507, 0.0018975332068311196,  
0.0019342359767891683, 0.0018115942028985507,  
0.0017543859649122807, 0.0016207455429497568,  
0.0015290519877675841, 0.0014492753623188406,  
0.0013157894736842105, 0.001375515818431912,  
0.0013175230566534915, 0.001466275659824047,  
0.0013054830287206266, 0.0013513513513513514,  
0.00145985401459854, 0.001451378809869376, 0.001388888888888889,  
0.001422475106685633, 0.0016233766233766235,  
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0.0014577259475218659, 0.0016366612111292963,  
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0.0013089005235602095, 0.0011494252873563218,  
0.0010672358591248667, 0.0010672358591248667,  
0.001277139208173691, 0.0013458950201884253,  
0.001567398119122257, 0.001524390243902439,  
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0.0014326647564469914, 0.0015600624024961,  
0.0013774104683195593, 0.001366120218579235,  
0.0015698587127158557, 0.0015625, 0.0016863406408094434,  
0.0017667844522968198, 0.0016233766233766235,  
0.0015772870662460567, 0.0017271157167530224,  
0.0016501650165016502, 0.0015151515151515152,  
0.0015037593984962407, 0.0015384615384615385,

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0.0011862396204033216, 0.001183431952662722,  
0.0012531328320802004, 0.001091703056768559,  
0.0011160714285714285, 0.0010298661174047373,  
0.001148105625717566, 0.0011467889908256881,  
0.0011876484560570072, 0.0010834236186348862,  
0.0011261261261261261, 0.001122334455667789,  
0.0010857763300760044, 0.0010799136069114472,  
0.0011737089201877935, 0.0011806375442739079,  
0.0013458950201884253, 0.0013717421124828531,  
0.0012578616352201257, 0.0014792899408284023,  
0.0014184397163120568, 0.001447178002894356,  
0.0014970059880239522]