

GPCR BOUND VS UNBOUND STATE ANALYSIS

PDB USED - 1R8Q.PDB – BOUND STATE

nodes = 249

average degree = 7.26104417671

avg clustering coeff = 0.564308248646

edges = 904

average shortest path = 5.95203394222

BETWEENNESS CENTRALITY =

[0, 0, 235, 21, 536, 876, 0, 329, 322, 0, 55, 407, 0, 155, 220, 158, 244, 482, 607, 392, 448, 222, 536, 424, 202, 0, 77, 247, 572, 98, 69, 282, 178, 205, 188, 254, 246, 818, 0, 279, 0, 434, 114, 220, 74, 232, 44, 375, 406, 876, 178, 233, 180, 269, 634, 413, 157, 353, 0, 206, 228, 332, 230, 268, 247, 273, 186, 233, 0, 345, 226, 65, 0, 585, 169, 73, 312, 404, 177, 263, 116, 613, 0, 284, 674, 299, 327, 199, 373, 386, 1006, 381, 541, 405, 526, 228, 0, 0, 136, 162, 16, 13, 1262, 253, 221, 98, 236, 76, 188, 0, 532, 38, 262, 0, 259, 669, 0, 32, 177, 590, 298, 251, 300, 408, 529, 389, 362, 85, 88, 8, 0, 13, 151, 87, 58, 649, 4, 23, 534, 248, 0, 70, 220, 216, 134, 0, 33, 451, 0, 11, 530, 73, 76, 40, 116, 488, 209, 364, 292, 296, 0, 0, 371, 0, 508, 116, 138, 38, 542, 98, 368, 96, 93, 403, 151, 152, 0, 401, 0, 137, 223, 277, 7, 91, 892, 166, 72, 673, 140, 255, 96, 79, 111, 589, 98, 41, 482, 220, 396, 242, 176, 555, 17, 681, 348, 0, 38, 158, 401, 102, 307, 8, 362, 194, 426, 0, 764, 371, 254, 237, 605, 140, 0, 0, 0, 119, 58, 134, 465, 15, 76, 228, 122, 33, 241, 170, 23, 38, 607, 437, 0, 39, 262, 170, 86, 160, 245, 492, 0, 0]

CLOSENESS CENTRALITY =

[0, 0.0005614823133071309, 0.0006455777921239509, 0.0006501950585175553, 0.0006920415224913495, 0.0007183908045977011, 0.0006527415143603133, 0.0006775067750677507, 0.0006447453255963894, 0.0006365372374283895, 0.0005820721769499418, 0.0006222775357809583, 0.0005963029218843172, 0.0006591957811470006, 0.0006657789613848203, 0.0007342143906020558, 0.0007587253414264037, 0.000855431993156544, 0.0008865248226950354, 0.0009082652134423251, 0.0008976660682226212, 0.0009049773755656109, 0.00088261253309797,

0.0008064516129032258, 0.0007309941520467836,
0.0007047216349541931, 0.0006743088334457181,
0.0007656967840735069, 0.0007727975270479134,
0.0007692307692307692, 0.0006978367062107466,
0.0007127583749109052, 0.000724112961622013,
0.0007507507507507507, 0.000725689404934688,
0.000741839762611276, 0.0007320644216691069,
0.0007886435331230284, 0.0006988120195667365,
0.0007092198581560284, 0.0006863417982155113,
0.0006613756613756613, 0.0006009615384615385,
0.0006289308176100629, 0.0005777007510109763,
0.0006242197253433209, 0.0006035003017501509,
0.0006811989100817438, 0.0006557377049180328,
0.0007423904974016332, 0.0007347538574577516,
0.0007818608287724785, 0.0007867820613690008,
0.0008417508417508417, 0.000877963125548727,
0.0008460236886632825, 0.0008210180623973727,
0.0007757951900698216, 0.0007423904974016332,
0.0007587253414264037, 0.0008143322475570033,
0.0008726003490401396, 0.0008920606601248885,
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0.0007052186177715092, 0.0006858710562414266,
0.0006949270326615705, 0.0006544502617801048,
0.0007102272727272727, 0.0007022471910112359,
0.0007032348804500703, 0.000725689404934688,
0.0007507507507507507, 0.0007535795026375283,
0.0007686395080707148, 0.000774593338497289,
0.0008264462809917355, 0.0008110300081103001,
0.0008244023083264633, 0.00088261253309797,
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0.0008291873963515755, 0.0008116883116883117,
0.0008136696501220504, 0.0008, 0.000723589001447178,
0.0007137758743754461, 0.0006353240152477764,
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0.0007132667617689016, 0.000715307582260372,
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0.0006756756756756757, 0.0006277463904582549,
0.000676132521974307, 0.0006253908692933083,
0.0006195786864931846, 0.0005834305717619603,
0.0006157635467980296, 0.0006226650062266501,
0.0005773672055427252, 0.0005678591709256105,
0.0006056935190793458, 0.0005506607929515419,
0.0005602240896358543, 0.0006090133982947625,
0.0005707762557077625, 0.0005589714924538849,
0.0005820721769499418, 0.0005977286312014345,
0.0005737234652897303, 0.000574052812858783,
0.0006211180124223603, 0.0006269592476489029,
0.0005621135469364812, 0.0005621135469364812,
0.0006273525721455458, 0.0005861664712778429,
0.0005467468562055768, 0.0005724098454493417,
0.0005122950819672131, 0.00045392646391284613,
0.0004083299305839118, 0.0004083299305839118]

PDB USED – 1RRF.PDB – UNBOUND STATE

nodes = 175

average degree = 7.37142857143
avg clustering coeff = 0.561054945055
edges = 645
average shortest path = 4.62568144499

BETWEENNESS CENTRALITY =

[0, 0, 147, 36, 386, 289, 78, 222, 227, 101, 0, 107, 156, 107, 32, 103, 155, 339, 427, 267, 460, 183, 505, 440, 184, 0, 94, 269, 172, 341, 85, 186, 239, 0, 62, 108, 304, 81, 413, 107, 48, 158, 51, 88, 46, 354, 0, 4, 0, 0, 3, 481, 266, 239, 113, 319, 237, 0, 0, 380, 117, 129, 199, 132, 206, 272, 44, 584, 0, 489, 0, 0, 27, 151, 300, 41, 0, 0, 236, 294, 0, 43, 468, 220, 116, 310, 239, 280, 386, 267, 334, 297, 211, 137, 0, 11, 173, 63, 11, 18, 866, 276, 62, 434, 136, 103, 0, 87, 298, 45, 47, 0, 26, 453, 0, 31, 158, 403, 214, 489, 178, 261, 398, 393, 322, 76, 56, 19, 0, 24, 137, 110, 11, 685, 53, 118, 118, 165, 0, 0, 340, 194, 124, 0, 37, 260, 0, 13, 358, 57, 12, 10, 72, 239, 80, 452, 217, 194, 0, 0, 154, 0, 238, 61, 161, 19, 221, 37, 193, 16, 804, 308, 0, 0, 0, 33]

CLOSENESS CENTRALITY =

[0, 0.0009074410163339383, 0.0010482180293501049, 0.001075268817204301, 0.001184834123222749, 0.0011614401858304297, 0.0011074197120708748, 0.001183431952662722, 0.0011534025374855825, 0.0010718113612004287, 0.0010384215991692627, 0.0010460251046025104, 0.0010893246187363835, 0.001072961373390558, 0.0010787486515641855, 0.0011337868480725624, 0.001215066828675577, 0.0013440860215053765, 0.0014285714285714286, 0.0015128593040847202, 0.0016155088852988692, 0.001607717041800643, 0.0016863406408094434, 0.0016313213703099511, 0.0014641288433382138, 0.0013774104683195593, 0.0013679890560875513, 0.0014858841010401188, 0.001321003963011889, 0.0014326647564469914, 0.0012285012285012285, 0.0012674271229404308, 0.0013315579227696406, 0.0013003901170351106, 0.0011792452830188679, 0.0012468827930174563, 0.0012674271229404308, 0.001201923076923077, 0.0012578616352201257, 0.0012406947890818859, 0.0011862396204033216,

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0.0011574074074074073, 0.0011325028312570782,
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0.0013440860215053765, 0.001326259946949602,
0.0013192612137203166, 0.0012919896640826874,
0.0012033694344163659, 0.0011198208286674132,
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0.0010141987829614604, 0.0010256410256410256,
0.0012239902080783353, 0.0010471204188481676,
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0.0016420361247947454, 0.0016722408026755853,
0.0017064846416382253, 0.0016835016835016834,
0.001610305958132045, 0.0014144271570014145,
0.00141643059490085, 0.0012360939431396785,
0.0012091898428053204, 0.001128668171557562,
0.0010857763300760044, 0.0012033694344163659,
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0.0012594458438287153, 0.001466275659824047,
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0.001375515818431912, 0.0013351134846461949,
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0.0012004801920768306, 0.001256281407035176,
0.0010964912280701754, 0.0011668611435239206,
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0.0013245033112582781, 0.0014265335235378032,
0.0014992503748125937, 0.0015503875968992248,

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0.0016129032258064516, 0.001607717041800643,
0.0015698587127158557, 0.0013717421124828531,
0.0013513513513513514, 0.0011494252873563218,
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0.0010570824524312897, 0.0012121212121212121,
0.0012330456226880395, 0.0011737089201877935,
0.0013908205841446453, 0.0011655011655011655,
0.001177856301531213, 0.0012254901960784314,
0.0012239902080783353, 0.0011185682326621924,
0.0010893246187363835, 0.0012121212121212121,
0.0011086474501108647, 0.0011507479861910242,
0.0010245901639344263, 0.0010256410256410256,
0.0011261261261261261, 0.0010672358591248667,
0.001098901098901099, 0.0012484394506866417,
0.0012738853503184713, 0.0013774104683195593,
0.0014492753623188406, 0.0014727540500736377,
0.001488095238095238, 0.001445086705202312,
0.0014814814814814814, 0.0013477088948787063,
0.0013850415512465374, 0.0011695906432748538,
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0.0012674271229404308, 0.0013513513513513514,
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0.0011806375442739079, 0.0013175230566534915,
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0.0012195121951219512, 0.0013986013986013986,
0.0012610340479192938, 0.0011904761904761906,
0.0011876484560570072, 0.001184834123222749,
0.0010799136069114472]