PDB USED - 1HQ2.PDB - bound state of 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase

```
nodes = 158
average degree = 7.72151898734
avg clustering coeff = 0.544386450399
edges = 610
average shortest path = 4.42562283319
```

BETWEENNESS CENTRALITY

NODE 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24	NO	0 165 157 304 378 286 355 280 328 653 334 114 0 30 321 11 25 430 95 61 82 159 98 46	VALUE
29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46		200 0 56 247 98 156 0 187 74 301 29 217 270 134 272 142 282 52	

47 48 49 50 51 52 53 54	46 90 39 0 123 43 145 235 301 192 360
48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 77 78 79 80 81 82 83	360 320 122 242 253 52 190 80 195 49
68 69 70 71 72 73 74 75 76 77	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
84 85 86 87 88 89	140 124
90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106	45 24 37 0 101 319 144 324 177 203 49 372 35 158 337 250 237 0 295 66 73

107 89	7
108 15 109 37	1
109 37 110 0 111 0 112 12	1
112 113 114 49	1
115 0	
116 29 117 0 118 69	
119 24 120 0	6
119 24 120 0 121 35 122 17 123 16 124 29	3
123 16 124 29 125 33	4
125 33 126 12	4
127 30 128 21 129 11	2
130 21 131 65	0
125 33 126 12 127 30 128 21 129 11 130 21 131 65 132 14 133 24	8
134 10	8
135 10 136 65 137 11	3
138 48 139 82	3
139 82 140 0 141 0 142 0	
	9
145 87 146 66	J
147 46 148 22	3
149 0 150 0	
152 12	7
153 31 154 75	4
155 37 156 20 157 54	7
157 54 158 0 159 0	

CLOSENESS CENTRALITY

NODE NO	VALUE
1	0
2	0.0014880952381

```
3
            0.0016077170418
4
            0.00170648464164
5
            0.00183823529412
6
            0.0019267822736
7
            0.00202429149798
8
            0.00194552529183
9
            0.00196078431373
10
            0.00184501845018
11
            0.0017094017094
12
            0.00151515151515
13
            0.00137551581843
14
            0.00138888888889
15
            0.00161812297735
16
            0.00138312586445
17
            0.00139664804469
18
            0.0016051364366
19
            0.00157480314961
20
            0.00138312586445
21
            0.00139275766017
22
            0.0014245014245
23
            0.00143266475645
2.4
            0.00133155792277
25
            0.0013986013986
26
            0.00134770889488
27
            0.00148588410104
28
            0.00127226463104
29
            0.00138121546961
30
            0.00125786163522
31
            0.00131233595801
32
            0.0014450867052
33
            0.00148367952522
34
            0.00155520995334
35
            0.00149476831091
36
            0.00162337662338
37
            0.00164473684211
38
            0.00175131348511
39
            0.0016051364366
40
            0.00170068027211
41
            0.00170357751278
42
            0.00158478605388
43
            0.00166112956811
            0.00149476831091
44
4.5
            0.00149031296572
46
            0.00125470514429
47
            0.00125313283208
48
            0.00120627261761
49
            0.00125
50
            0.00111234705228
51
            0.00132450331126
52
            0.00141843971631
53
            0.00157232704403
54
            0.00172117039587
55
            0.00184501845018
56
            0.0018691588785
57
            0.00195694716243
58
            0.00190476190476
59
            0.0018315018315
60
            0.00174825174825
61
            0.00165289256198
62
            0.00153609831029
```

```
63
            0.00147710487445
64
            0.00134228187919
65
            0.00134408602151
66
            0.00126903553299
67
            0.00121802679659
68
            0.00119474313023
69
            0.00125628140704
70
            0.00139470013947
71
            0.00137174211248
72
            0.00137362637363
73
            0.0014367816092
74
            0.00166389351082
75
            0.00142857142857
76
            0.00142653352354
77
            0.00148367952522
78
            0.00170357751278
79
            0.00144717800289
80
            0.00141242937853
            0.00152671755725
81
82
            0.00146627565982
83
            0.0015243902439
84
            0.00135501355014
85
            0.00125628140704
86
            0.00115074798619
87
            0.00107991360691
88
            0.0011273957159
89
            0.00112233445567
90
            0.00121654501217
91
            0.00133511348465
92
            0.00142045454545
93
            0.00161812297735
94
            0.00161030595813
95
            0.00179533213645
96
            0.0018115942029
97
            0.00196463654224
98
            0.0018281535649
99
            0.00185873605948
100
            0.0018018018018
101
            0.0017094017094
102
            0.0016155088853
103
            0.00151515151515
104
            0.00149253731343
105
            0.00136612021858
106
            0.00133868808568
107
            0.00129701686122
108
            0.00129533678756
109
            0.00115074798619
110
            0.00108225108225
111
            0.00105596620908
112
            0.00126103404792
113
            0.00135135135135
114
            0.0015455950541
115
            0.00150829562594
116
            0.00162601626016
117
            0.00141843971631
118
            0.00145348837209
119
            0.0015873015873
120
            0.00140845070423
121
            0.00138504155125
122
            0.00159744408946
```

123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155	0.00158478605388 0.00174216027875 0.0017825311943 0.00168067226891 0.00163132137031 0.00177304964539 0.00166666666667 0.00157232704403 0.00152905198777 0.00156985871272 0.0014367816092 0.00139275766017 0.00125156445557 0.00130548302872 0.00125628140704 0.00136054421769 0.00128865979381 0.00114155251142 0.00115340253749 0.0012315270936 0.00124378109453 0.00124378109453 0.00124378109453 0.00124378109453 0.00123399020808 0.00118063754427 0.00118203309693 0.00126742712294 0.00113250283126 0.0011013215859 0.00122549019608 0.00129198966408 0.00129198966408
154	0.00129198966408

PDB USED - 1IM6.PDB - unbound state of 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase

```
nodes = 158
average degree = 7.50632911392
avg clustering coeff = 0.554656770796
edges = 593
average shortest path = 4.54906071112
```

BETWEENNESS CENTRALITY

NODE	NO	0	VALUE
1 2 3 4 5 6		100	
3		207 248	
		381 305	
7 8		343 308	
9 10		231 596	
11 12		328 158	
13		0	
14 15		32 416	
16 17		11 36	
18 19		13 383	
20 21		58 125	
22 23		52 130	
24		41	
25 26		265 0	
27 28		496 48	
29 30		68 0	
31 32		49 340	
33 34		49 160	
35 36		0 173	
37		65	
38 39		299 129	
40 41		121 274	
42 43		198 127	
44 45		150 179	
46		111	

47 47 47 49 90 12 34 56 66 66 66 66 66 67 77 77 77 77 77 77 77	6 4 2 131 86 262 110 326 340 218 347 390 1251 37 42 96 18 374 286 175 69 28 91 479 50 15 230 496 10 61 41 61 61 61 61 61 61 61 61 61 61 61 61 61
99	146

107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 130 131 132 133 134 145 146 147 148 149 149 159 169 169 169 169 169 169 169 169 169 16	98 0 76 0 0 240 153 475 44 285 0 63 238 171 258 2381 381 257 141 101 110 264 142 100 262 319 45 395 0 0 387 42 227 90 90 90 90 90 90 90 90 90 90
156 157 158 159	10 0 0

CLOSENESS CENTRALITY

NODE	NO	VALUE
1		0
2		0.00143061516452

```
3
            0.00157480314961
4
            0.00168067226891
5
            0.00181488203267
6
            0.00188323917137
7
            0.00197628458498
8
            0.00190114068441
9
            0.00188679245283
10
            0.00181488203267
11
            0.00157232704403
12
            0.00153609831029
13
            0.00134048257373
14
            0.00134228187919
15
            0.00155763239875
16
            0.00130548302872
17
            0.00133868808568
18
            0.00134228187919
19
            0.00152671755725
20
            0.00131406044678
21
            0.00134770889488
22
            0.00134770889488
23
            0.00142857142857
2.4
            0.00133333333333
25
            0.00140252454418
26
            0.00133333333333
27
            0.00149031296572
28
            0.00127388535032
29
            0.00135317997294
30
            0.00124843945069
31
            0.00130039011704
32
            0.00145772594752
33
            0.00148148148148
34
            0.00155520995334
35
            0.00148367952522
36
            0.00159744408946
37
            0.00161030595813
38
            0.00172711571675
39
            0.00162866449511
40
            0.00167785234899
41
            0.00166389351082
42
            0.00154320987654
43
            0.0015243902439
44
            0.00139275766017
4.5
            0.001287001287
46
            0.00115874855156
47
            0.00107874865156
48
            0.00101214574899
49
            0.00104384133612
50
            0.00116009280742
51
            0.00123762376238
52
            0.00140252454418
53
            0.00151057401813
54
            0.00168067226891
55
            0.00178890876565
56
            0.0018115942029
57
            0.00189753320683
58
            0.00193423597679
59
            0.0018115942029
60
            0.00175438596491
61
            0.00162074554295
62
            0.00152905198777
```

```
63
            0.00144927536232
64
            0.00131578947368
65
            0.00137551581843
66
            0.00131752305665
67
            0.00146627565982
68
            0.00130548302872
69
            0.00135135135135
70
            0.0014598540146
71
            0.00145137880987
72
            0.00138888888889
73
            0.00142247510669
74
            0.00162337662338
75
            0.00144717800289
76
            0.00140252454418
77
            0.00145772594752
78
            0.00163666121113
79
            0.00142857142857
80
            0.00138888888889
81
            0.00139470013947
82
            0.0014598540146
83
            0.00136612021858
84
            0.00126422250316
85
            0.00114810562572
86
            0.00114547537228
87
            0.00115207373272
88
            0.00115340253749
89
            0.00114810562572
90
            0.00110497237569
91
            0.00132450331126
92
            0.00128865979381
93
            0.00136798905609
94
            0.0015923566879
95
            0.00169779286927
96
            0.0017667844523
97
            0.00186567164179
98
            0.0017793594306
99
            0.00176056338028
100
            0.00177619893428
101
            0.00162074554295
102
            0.00162866449511
103
            0.00147928994083
104
            0.00138696255201
105
            0.0013986013986
106
            0.00134952766532
107
            0.00131578947368
108
            0.00130890052356
109
            0.00114942528736
110
            0.00106723585912
111
            0.00106723585912
112
            0.00127713920817
113
            0.00134589502019
            0.00156739811912
114
115
            0.0015243902439
116
            0.0015873015873
117
            0.00137931034483
118
            0.00143266475645
119
            0.0015600624025
120
            0.00137741046832
121
            0.00136612021858
122
            0.00156985871272
```

123 124 125 126 127 128 129	0.0015625 0.00168634064081 0.0017667844523 0.00162337662338 0.00157728706625 0.00172711571675 0.0016501650165 0.00151515151515
131 132	0.001513131313 0.0015037593985 0.00153846153846
133	0.00142045454545
134	0.00135685210312
135	0.00124533001245
136	0.00126422250316
137	0.0011862396204
138 139	0.0011802330204 0.00118343195266 0.00125313283208
140	0.00109170305677
141	0.00111607142857
142	0.0010298661174
143	0.00114810562572
144	0.00114678899083
144	0.00114678899083
145	0.00118764845606
146	0.00108342361863
147	0.00112612612613
148	0.00112233445567
149	0.00108577633008
150	0.00107991360691
151	0.00117370892019
152	0.00118063754427
153	0.00134589502019
154	0.00137174211248
155	0.00125786163522
156	0.00147928994083
157	0.00141843971631
158	0.00144717800289
159	0.00144717800289