Table S1: Systems with problems detected by Prepscript

Problem	System
Incomplete side chains	
Bound complexes	1A2K, 1AVX, 1BGX, 1D6R,[a] 1DE4, 1E6E, 1E96,[a] 1EER,[c] 1EWY, 1EZU, 1F51, 1FC2, 1GHQ, 1GRN,[a] 1I4D, 1IBR,[c] 1IJK, 1IQD, 1K4C, 1KKL, 1KXQ, 1MAH,[a] 1N2C, 1QFW, 1SBB, 1WQ1, 2HMI,[c] 2JEL, 2QFW
Unbound complexes	1A2K,[b] 1ATN,[c] 1AVX, 1BGX,[b] 1BUH, 1D6R,[a] 1DE4,[c] 1E96,[a] 1EZU, 1F51, 1FAK,[c] 1FC2,[b] 1GP2,[a,b] 1GRN,[a] 1H1V,[c] 1HE1,[a] 1HIA,[a,b] 1I2M,[a] 1I4D,[b] 1IB1,[b] 1IBR,[c] 1IJK, 1IQD, 1K4C, 1KKL,[b] 1KLU,[b] 1KXQ, 1KXP,[a] 1M10,[a,b] 1MAH,[a] 1N2C,[b] 1NSN, 1QFW, 1SBB, 2JEL, 2PCC,[a] 2QFW
Cofactors not defined in charge library	1E6E (FAD), 1EWY (FAD), 1HE8_u (GTN), 1IB1 (COT), 1RLB (REA, RTL), 1TMQ (5HP), 1WQ1_u (GCP)
Problems with protonation	1VFB_u, 2QFW_b
Needed huge grid	1EER,[c] 2VIS_u (Moving molecule has twice the maximum dimension in unbound (135 Å) than in bound (71 Å) coordinates)
Large total charge	1ML0 (-42 for receptor)

[a] Dot was run on these systems and the results are in Table 1.

[b] Systems on which ZDOCK was run, but no correct answers were found.

[c] Systems ranked 'difficult' in Benchmark 2.0, no ZDOCK runs.