Similarity clustering ../run_2.1/Final/M00000328_FIT.sdf ../run_4.0/Final/M00000145_FIT.sdf ../run_3.0/Final/M00000207_FIT.sdf ../run_3.0/Final/M00000240 FIT.sdf ../run 3.0/Final/M00000238 FIT.sdf ../run_4.0/Final/M00000180_FIT.sdf ../run_4.1/Final/M00000205_FIT.sdf ../run_4.1/Final/M00000231 FIT.sdf ../run_4.1/Final/M00000217_FIT.sdf ../run_2.2/Final/M00000092_FIT.sdf ../run_2.2/Final/M00000085_FIT.sdf ../run_2.2/Final/M00000200_FIT.sdf ../run_2.2/Final/M00000190_FIT.sdf ../run_2.2/Final/M00000144_FIT.sdf ../run_2.2/Final/M00000097_FIT.sdf ../run_2.1/Final/M00000263_FIT.sdf ../run_2.1/Final/M00000301_FIT.sdf ../run_2.2/Final/M00000113 FIT.sdf ../run_2.2/Final/M00000099_FIT.sdf ../run_2.2/Final/M00000087_FIT.sdf ../run 2.1/Final/M00000267 FIT.sdf ../run_2.1/Final/M00000245_FIT.sdf ../run 2.2/Final/M00000046 FIT.sdf ../run_2.1/Final/M00000309_FIT.sdf ../run_2.1/Final/M00000298_FIT.sdf ../run 2.1/Final/M00000259 FIT.sdf ../run_2.1/Final/M00000308_FIT.sdf ../run 2.2/Final/M00000160 FIT.sdf ../run_2.2/Final/M00000174_FIT.sdf ../run_2.2/Final/M00000105_FIT.sdf ../run_2.2/Final/M00000141_FIT.sdf ../run_2.2/Final/M00000202_FIT.sdf ../run_4.0/Final/M00000214_FIT.sdf ../run_2.1/Final/M00000182_FIT.sdf ../run_2.1/Final/M00000258_FIT.sdf ../run_2.1/Final/M00000253_FIT.sdf ../run_2.1/Final/M00000178_FIT.sdf ../run_2.2/Final/M00000180_FIT.sdf ../run_2.1/Final/M00000193_FIT.sdf ../run_2.1/Final/M00000275_FIT.sdf ../run_2.1/Final/M00000243_FIT.sdf ../run_2.1/Final/M00000157_FIT.sdf ../run_2.1/Final/M00000201_FIT.sdf ../run_2.1/Final/M00000284_FIT.sdf ../run_2.1/Final/M00000322_FIT.sdf ../run_2.1/Final/M00000257_FIT.sdf ../run 2.1/Final/M00000295 FIT.sdf ../run_2.2/Final/M00000183 FIT.sdf ../run_2.2/Final/M00000101_FIT.sdf ../run 2.1/Final/M00000116 FIT.sdf ../run_2.1/Final/M00000107_FIT.sdf ../run 4.1/Final/M00000075 FIT.sdf ../run_4.0/Final/M00000217_FIT.sdf ../run_4.0/Final/M00000200_FIT.sdf ../run_2.1/Final/M00000292_FIT.sdf ../run_4.0/Final/M00000097_FIT.sdf ../run_4.0/Final/M00000174_FIT.sdf ../run_4.0/Final/M00000137_FIT.sdf ../run_4.0/Final/M00000222_FIT.sdf ../run_4.0/Final/M00000216_FIT.sdf ../run_2.0/Final/M00000482_FIT.sdf ../run_2.0/Final/M00000512_FIT.sdf ../run_2.0/Final/M00000386_FIT.sdf ../run_2.0/Final/M00000217_FIT.sdf ../run_2.0/Final/M00000181_FIT.sdf ../run_1.1/Final/M00000254_FIT.sdf ../run 2.0/Final/M00000459 FIT.sdf ../run_2.0/Final/M00000362_FIT.sdf ../run_1.1/Final/M00000332_FIT.sdf ../run_2.0/Final/M00000410_FIT.sdf ../run_2.0/Final/M00000317_FIT.sdf ../run 2.0/Final/M00000285 FIT.sdf ../run_2.0/Final/M00000167_FIT.sdf ../run_1.1/Final/M00000299_FIT.sdf ../run_1.1/Final/M00000267_FIT.sdf ../run_2.0/Final/M00000179_FIT.sdf ../run 1.1/Final/M00000274 FIT.sdf ../run_2.0/Final/M00000340 FIT.sdf ../run_1.1/Final/M00000359_FIT.sdf ../run_1.1/Final/M00000318_FIT.sdf ../run_1.1/Final/M00000288_FIT.sdf ../run 1.1/Final/M00000320 FIT.sdf ../run_1.1/Final/M00000302_FIT.sdf ../run_1.1/Final/M00000297_FIT.sdf ../run 1.1/Final/M00000289 FIT.sdf ../run_1.1/Final/M00000310_FIT.sdf ../run 1.1/Final/M00000300 FIT.sdf ../run 1.1/Final/M00000281 FIT.sdf ../run_2.0/Final/M00000545_FIT.sdf ../run 1.1/Final/M00000330 FIT.sdf /run 2.0/Final/M00000407 FIT.sdf ../run 2.0/Final/M00000472 FIT.sdf ../run_1.1/Final/M00000370 FIT.sdf ../run_1.1/Final/M00000381 FIT.sdf ../run_2.0/Final/M00000258_FIT.sdf ../run 2.0/Final/M00000228 FIT.sdf ../run 1.1/Final/M00000401 FIT.sdf ../run_1.1/Final/M00000369 FIT.sdf ../run_1.1/Final/M00000306_FIT.sdf ../run_2.0/Final/M00000370_FIT.sdf ../run 1.1/Final/M00000340 FIT.sdf ../run 1.1/Final/M00000341 FIT.sdf ../run_1.1/Final/M00000405_FIT.sdf ../run_4.1/Final/M00000200 FIT.sdf ../run 1.1/Final/M00000406 FIT.sdf ../run_2.0/Final/M00000214_FIT.sdf ../run 2.0/Final/M00000306 FIT.sdf 1.4 1.2 1.0 8.0 0.6 0.4 0.2 0.0