Prime energies for various structures of 2H59 in Loop refinement

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| **Sir2TM H116A mutant ternary complex loop refinement** | **MM-GBSA** |
| step 1: protein preparation wizard | -10964.2 |
| minimizing res 37-42 + 7.5 Å after step 1 | -11041.8 |
| minimizing res 37-44 + 7.5 Å after step 1 | -11053.9 |
| minimizing res 35-46 + 7.5 Å after step 1 | -11087.4 |
| minimizing res 33-47 + 7.5 Å after step 1 | -11137.7 |
| full minimization | -11634.6 |
| Job 1: loop refinement on res 37-42 after step 1; extended sampling | -10999.6 |
| energy extracted from log file of Job 1 | -10999.6307 |
| energy calculation of rank 1 structure from Loop Refinement Job 1 | -10999.55896 |
| energy calculation of rank 1 structure from Loop Refinement Job 1 on gpu1 | -10999.55881 |
| reminimization of rank 1 structure from Loop Refinement Job 1 | -11002.8 |
| Full minimization of rank 1 from Loop Refinement Job 1 |  |
| Job 2: loop refinement on res 37-44 after step 1; extended sampling | -10989.7 |
| Job 3: loop refinement on res 35-46 after step 1; extended sampling | -10981.3 |
| Job 4: loop refinement on res 33-47 after step 1; extended sampling | -10982.2 |
| Job 5: loop refinement on res 33-47 after step 1; ultra extended sampling | -10998.6 |
| Job 6: loop refinement on res 33-47 after step 1; modified ultra extended sampling, 5 initial stages | -11005.1 |
| Job 7: loop refinement on res 33-47 after step 1; modified ultra extended sampling, 5 initial stages, 10 fixed stages | -11024.5 |
| Job 8: loop refinement on res 36-43 after step 1; extended sampling | -11003.7 |
| Job 9: loop refinement on res 36-45 after step 1; extended sampling | -10981.9 |
| Job 10: loop refinement on res 36-43 after step 1; extended sampling, same input as Job 8, run on gpu1 | -11008.6 |
| Job 11: loop refinement on res 36-45 after step 1; extended sampling, same input as Job 9, run on gpu1 | -10987.8 |
| Job 12: loop refinement on res 36-45 after step 1; modified extended sampling, 11 initial stages, run on gpu1 | -10986.2 |
| Job 13: loop refinement on res 37-44 after step 1; ultra extended sampling (actually 4 fixed stages) | -11012.7 |
| Job 14: loop refinement on res 37-44 after step 1; modified ultra extended sampling, 5 initial stages, 10 fixed stages (actually 4 fixed stages) | -11012.6 |
| Job 15: loop refinement on res 35-46 after step 1; ultra extended sampling (actually 5 fixed stages) | -11000 |
| Job 16: loop refinement on res 35-46 after step 1; modified ultra extended sampling, 5 initial stages, 10 fixed stages (actually 8 fixed stages) | -11002.5 |
| Job 17: loop refinement on res 36-45 after step 1; ultra extended sampling (actually 5 fixed stages) | -10994.4 |
| Job 18: loop refinement on res 36-45 after step 1; modified ultra extended sampling, 5 initial stages, 10 fixed stages (actually 8 fixed stages) | -11002.6 |
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| minimizing res 37-42 only after step 1 | -10974.7 |
| minimizing res 37-42 + 7.5 Å matching sidechain after step 1 | -10983.4 |
| minimizing res 37-44 + 7.5 Å matching sidechain after step 1 | -10994.5 |
| minimizing res 35-46 + 7.5 Å matching sidechain after step 1 | -11000.4 |
| minimizing res 33-47 + 7.5 Å matching sidechain after step 1 | -11007.6 |
| minimizing res 36-43 + 7.5 Å matching sidechain after step 1 | -10995.9 |
| minimizing res 36-45 + 7.5 Å matching sidechain after step 1 | -10998.3 |