





Ceritinib, rotatable bonds, 67 conformations (26, 25)(25, 23)(19, 18) -(18, 4)(5, 14) -**Bond indices** (14, 15)(15, 16) -(15, 17)(7, 8)(2, 1)(31, 32)-(32, 35)(35, 36)(35, 37)0.85 0.90 0.95 1.00 1.05 1.10 1.15

Bond order

Ceritinib, ring bonds, 67 conformations (28, 27)(28, 29)(29, 30)(30, 31)(31, 26)(26, 27)(23, 24)(23, 22)(22, 21)**Bond indices** (21, 20)(20, 19)(19, 24)(4, 5)(4, 3)(3, 2)(2, 7)(7, 6)(6, 5)(8, 9)(8, 13) -(13, 12)(12, 11)(11, 10) -(10, 9)1.0 1.1 1.2 1.3 1.4

Bond order