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| --- | --- |
| CCDC number | 1988897 |
| Empirical formula | C13H11ClN4O2 |
| Formula weight | 290.711 |
| Temperature/K | 293(2) |
| Crystal system | monoclinic |
| Space group | P21/c |
| a/Å | 11.7767(7) |
| b/Å | 14.4529(7) |
| c/Å | 7.9073(4) |
| α/° | 90 |
| β/° | 91.381(5) |
| γ/° | 90 |
| Volume/Å3 | 1345.49(12) |
| Z | 4 |
| ρcalcg/cm3 | 1.435 |
| μ/mm‑1 | 0.291 |
| F(000) | 600.8 |
| Crystal size/mm3 | 0.540 × 0.496 × 0.356 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 6.76 to 55.62 |
| Index ranges | -8 ≤ h ≤ 14, -17 ≤ k ≤ 17, -8 ≤ l ≤ 10 |
| Reflections collected | 4639 |
| Independent reflections | 2650 [Rint = 0.0162, Rsigma = 0.0324] |
| Data/restraints/parameters | 2650/0/182 |
| Goodness-of-fit on F2 | 1.055 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0568, wR2 = 0.1302 |
| Final R indexes [all data] | R1 = 0.0890, wR2 = 0.1541 |
| Largest diff. peak/hole / e Å-3 | 0.29/-0.56 |