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| --- | --- |
| CCDC number | 1988897 |
| Empirical formula | C13H11ClN4O2 |
| Formula weight | 290.71 |
| 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) | 600.0 |
| Crystal size/mm3 | 0.14 × 0.13 × 0.12 |
| Radiation | Mo Kα (λ = 0.71073) |
| 2Θ range for data collection/° | 6.756 to 49.996 |
| Index ranges | -8 ≤ h ≤ 14, -16 ≤ k ≤ 16, -8 ≤ l ≤ 9 |
| Reflections collected | 4286 |
| Independent reflections | 2343 [Rint=0.0161, Rsigma = 0.0302] |
| Data/restraints/parameters | 2343/0/182 |
| Goodness-of-fit on F2 | 1.047 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0548, wR2 = 0.1338 |
| Final R indexes [all data] | R1 = 0.0790, wR2 = 0.1491 |
| Largest diff. peak/hole / e Å-3 | 0.21/-0.41 |