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(2*Z*)-3-(4-Chloroanilino)-1-(5-hydroxy-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)but-2-en-1-one

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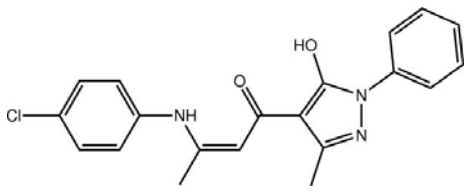
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.103; data-to-parameter ratio = 15.8.

With the exception of the terminal benzene rings, the atoms in the title compound, $C_{20}H_{18}ClN_3O_2$, are approximately coplanar (r.m.s. deviation = 0.0495 Å). The benzene/chlorobenzene rings form dihedral angles of 3.02 (4) and 41.59 (5)°, respectively, with this plane. The hydroxy, amino and carbonyl groups all lie to the same side of the molecule, enabling the formation of intramolecular O—H···O and N—H···O hydrogen bonds that close S(6) rings. The configuration about the 2-butene bond is Z. Supramolecular chains mediated by C—H···Cl interactions and aligned along the c axis are found in the crystal packing. These assemble into layers that are connected by weak π–π interactions between centrosymmetrically related chlorobenzene rings [3.8156 (9) Å].

Related literature

For background to the synthesis, see: Gelin *et al.* (1983); Bendaas *et al.* (1999).



Experimental

Crystal data

$C_{20}H_{18}ClN_3O_2$ M_r = 367.82
Monoclinic, $P2_1/n$
a = 10.7782 (3) Å
b = 12.6349 (4) Å
c = 12.9071 (4) Å
β = 100.956 (3)°
V = 1725.67 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.931, T_{max} = 0.953
8785 measured reflections
3860 independent reflections
3199 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.01
3860 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.96 (3)	1.64 (3)	2.5283 (16)	153 (3)
N3—H3···O2	0.91 (2)	1.93 (2)	2.6678 (18)	136.9 (18)
C4—H4···Cl1^{i}	0.95	2.81	3.6217 (18)	144

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{3}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5069).

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