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(*E*,*E*)-4-{4-[3-(4-Chloroanilino)-1-hydroxybut-2-enylidene]-3-methyl-5-oxo-4,5-dihydro-1*H*-pyrazol-1-yl}-benzenesulfonamide

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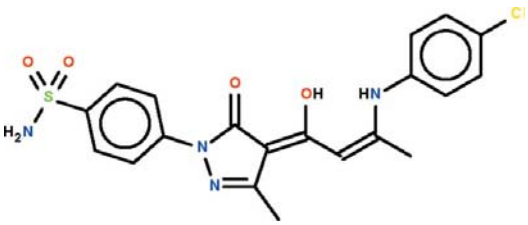
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.125; data-to-parameter ratio = 12.5.

The molecule of the title compound, $C_{20}H_{19}ClN_4O_4S$, features a central pyrazole ring that possesses a benzene substituent, as well as a conjugated ═C—C═C—C_{methyl} substituent. The benzene ring is slightly twisted [dihedral angle = 7.7 (2)°] with respect to the five-membered ring; the mean plane of the zigzag ═C—C═C—C fragment [torsion angle = 178.0 (4)°] is also slightly twisted [dihedral angle = 10.6 (4)°]. The amine and hydroxy groups form intramolecular hydrogen bonds. The amide group uses one of its H atoms to form a hydrogen bond to the sulfamyl O atom of an inversion-related molecule. Adjacent dimers are further linked by an N—$H_{amido}\cdots N_{pyrazole}$ hydrogen bond to generate a linear chain. The crystal studied is a nonmerohedral twin with a minor twin component of 25.6 (2)%.

Related literature

For the synthesis of 4-acetoacetyl-3-methyl-5-onyl-1-phenyl-pyrazole, see: Gelin *et al.* (1983).



Experimental

Crystal data

$C_{20}H_{19}ClN_4O_4S$
M_r = 446.90
Monoclinic, $P2_1/c$
a = 14.7513 (17) Å
b = 17.545 (2) Å
c = 7.6203 (9) Å
β = 101.496 (2)°
V = 1932.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 100 K
0.20 × 0.02 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (TWINABS; Bruker, 2009)
T_{min} = 0.935, T_{max} = 0.993
32586 measured reflections
3426 independent reflections
2605 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.125
S = 1.04
3426 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O2	0.84	1.79	2.498 (4)	141
N1—H1···O1	0.88	2.00	2.659 (4)	131
N1—H1···O3^{i}	0.88	2.34	3.093 (4)	143
N4—H41···N2^{ii}	0.88	2.16	3.003 (4)	161
N4—H42···O4^{iii}	0.88	2.09	2.917 (4)	156

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y, z-1$; (iii) $-x, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); 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: XU5227).

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