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(*E*)-4-[(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-ylimino)methyl]-phenyl 4-chlorobenzoate

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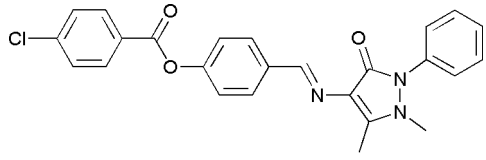
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.120; data-to-parameter ratio = 13.6.

In the title compound, $C_{25}H_{20}ClN_3O_3$, the central benzene ring makes dihedral angles of 7.56 (10), 39.46 (7) and 63.03 (7)° with the pyrazolone ring, the chlorobenzene ring and the terminal phenyl ring, respectively. The packing is stabilized by weak C—H···O intermolecular hydrogen bonds that link molecules into chains running along the *b* axis.

Related literature

For general background, see: Hu (2006); Kahwa *et al.* (1986); Klayman *et al.* (1979); Santos *et al.* (2001). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{25}H_{20}ClN_3O_3$
M_r = 445.89
Monoclinic, $C2/c$
a = 31.764 (7) Å
b = 6.7113 (16) Å
c = 25.605 (6) Å
β = 126.165 (3)°
V = 4406.7 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 294 (2) K
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.921, T_{max} = 0.960
10804 measured reflections
3962 independent reflections
2422 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 1.03
3962 reflections
292 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18C···O3^{i}	0.96	2.46	3.405 (3)	169
C19—H19A···O3^{i}	0.96	2.58	3.497 (3)	161
C2—H2···O3^{ii}	0.93	2.53	3.219 (3)	131

Symmetry codes: (i) $x, y-1, z$; (ii) $x, -y+2, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2534).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.
Hu, T.-P. (2006). *Acta Cryst.* E**62**, o2270–o2271.
Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.
Klayman, D. L., Bartosevich, J. F., Griffin, T. S., Mason, C. J. & Scovill, J. P. (1979). *J. Med. Chem.* **22**, 855–862.
Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2007). E**63**, o4035 [**doi:10.1107/S1600536807043796**]

(*E*)-4-[(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-ylimino)methyl]phenyl 4-chlorobenzoate

J.-R. Han, X.-L. Zhen, X. Tian, F. Li and S.-X. Liu

Comment

The synthesis and structure of Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.*, 1986 and Klayman *et al.*, 1979). Many Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics (Santos *et al.*, 2001). Among the large number of compounds, 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of them, such as (*E*)-4-[4-(4-Chlorobenzyloxy)benzylideneamino]-1,5- dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Hu, 2006) has been reported. Such structural information is useful when investigating the potential coordination properties of Schiff bases functioning as ligands. We new report the synthesis and molecular structure of the title Schiff base, (I), (Fig. 1)

In the title molecule (Fig. 1), the pyrazolone ring (C15—C17/N1/N2/N3/O3) is nearly planar, with an r.m.s. deviation for the fitted atoms of 0.038 Å. It makes a dihedral angle of 55.54 (7)° with its attached phenyl ring (C20—C25). The central benzene ring (C8—C14/O1) is almost planar, with an r.m.s. deviation for fitted atoms of 0.017 Å. This group makes dihedral angles of 7.56 (10)°, 39.46 (7)° and 63.03 (7)°, respectively, with the the pyrazolone ring (C15—C17/N1/N2/N3/O3), the terminal C1—C6 benzene ring and the terminal C20—C25 phenyl ring. Otherwise, all bond lengths and angles are within their normal ranges (Allen *et al.*, 1987).

The packing for (I) is stabilized by weak, non-classical intermolecular C—H···O hydrogen bonds that links molecules into one-dimensional extended chains running along the *b* axis (Fig. 2, Table 1).

Experimental

An anhydrous ethanol solution (50 ml) of 4-formylphenyl 4-chlorobenzoate (2.61 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture stirred at 350 K for 3 h under N_2, giving a yellow precipitate. The product was isolated, recrystallized from acetonitrile, and then dried in a vacuum to give pure compound (I) in 87% yield. Yellow blocks of (I) were obtained by slow evaporation of an acetonitrile solution.

Refinement

The H atoms were included in calculated positions and refined using a riding model approximation. Constrained C—H and N—H bond lengths and isotropic U parameters: 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H; 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene C—H; 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl C—H.

Figures

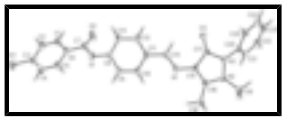

Fig. 1. The structure of (I) with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

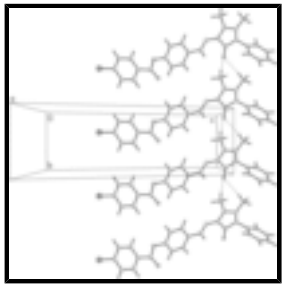

Fig. 2. Packing diagram for (I), with H bonds drawn as dashed lines.

(*E*)-4-[(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro −1*H*-pyrazol-4-ylimino)methyl]phenyl 4-chlorobenzoate

Crystal data

$C_{25}H_{20}ClN_3O_3$	F_{000} = 1856
M_r = 445.89	D_x = 1.344 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2545 reflections
a = 31.764 (7) Å	θ = 3.2–24.2º
b = 6.7113 (16) Å	μ = 0.21 mm^{-1}
c = 25.605 (6) Å	*T* = 294 (2) K
β = 126.165 (3)º	Block, yellow
V = 4406.7 (18) Å^3	0.26 × 0.24 × 0.20 mm
Z = 8	

Data collection

Bruker SMART APEX CCD diffractometer	3962 independent reflections
Radiation source: fine-focus sealed tube	2422 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 294(2) K	θ_{max} = 25.2º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −38→37
T_{min} = 0.921, T_{max} = 0.960	*k* = −8→5
10804 measured reflections	*l* = −30→29

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.120$

$S = 1.03$

3962 reflections

292 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.4018P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.23$ e Å^{-3}

$\Delta\rho_{min} = -0.21$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0009 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.02921 (3)	0.85943 (14)	0.32838 (3)	0.0868 (3)
O1	0.06375 (6)	0.6862 (2)	0.60622 (7)	0.0559 (5)
O2	0.10080 (8)	0.9908 (3)	0.62984 (8)	0.0897 (7)
O3	0.14117 (6)	0.6064 (2)	0.98425 (7)	0.0527 (4)
N1	0.14862 (7)	0.3501 (3)	0.88646 (8)	0.0454 (5)
N2	0.20831 (7)	0.1617 (3)	1.04555 (8)	0.0450 (5)
N3	0.18559 (7)	0.3329 (3)	1.05031 (8)	0.0423 (5)
C1	0.07274 (9)	1.0228 (4)	0.50268 (11)	0.0637 (7)
H1	0.0863	1.1358	0.5286	0.076*
C2	0.06193 (9)	1.0265 (5)	0.44201 (12)	0.0655 (7)
H2	0.0678	1.1410	0.4267	0.079*
C3	0.04222 (8)	0.8573 (4)	0.40467 (10)	0.0548 (7)
C4	0.03306 (9)	0.6874 (4)	0.42588 (11)	0.0567 (7)
H4	0.0200	0.5742	0.4000	0.068*
C5	0.04351 (8)	0.6865 (4)	0.48666 (10)	0.0526 (6)
H5	0.0369	0.5725	0.5013	0.063*
C6	0.06368 (8)	0.8535 (4)	0.52553 (10)	0.0475 (6)
C7	0.07797 (9)	0.8564 (4)	0.59202 (11)	0.0547 (7)
C8	0.07828 (8)	0.6511 (4)	0.66906 (10)	0.0477 (6)
C9	0.09811 (9)	0.4660 (4)	0.69396 (10)	0.0545 (6)
H9	0.1023	0.3739	0.6702	0.065*

C10	0.11186 (9)	0.4166 (4)	0.75437 (11)	0.0541 (6)
H10	0.1253	0.2907	0.7712	0.065*
C11	0.10592 (8)	0.5522 (4)	0.79049 (10)	0.0470 (6)
C12	0.08446 (9)	0.7354 (4)	0.76314 (11)	0.0601 (7)
H12	0.0790	0.8263	0.7860	0.072*
C13	0.07073 (9)	0.7882 (4)	0.70247 (11)	0.0602 (7)
H13	0.0568	0.9131	0.6850	0.072*
C14	0.12225 (8)	0.5065 (4)	0.85623 (10)	0.0507 (6)
H14	0.1132	0.5936	0.8763	0.061*
C15	0.16474 (8)	0.3141 (3)	0.94963 (10)	0.0391 (5)
C16	0.19226 (8)	0.1468 (3)	0.98340 (10)	0.0422 (5)
C17	0.16029 (8)	0.4388 (3)	0.99142 (10)	0.0398 (5)
C18	0.20356 (9)	−0.0335 (4)	0.96011 (11)	0.0579 (7)
H18A	0.2406	−0.0542	0.9857	0.087*
H18B	0.1902	−0.0158	0.9156	0.087*
H18C	0.1872	−0.1472	0.9640	0.087*
C19	0.21951 (10)	−0.0063 (4)	1.08845 (11)	0.0638 (7)
H19A	0.1937	−0.1081	1.0646	0.096*
H19B	0.2189	0.0382	1.1236	0.096*
H19C	0.2534	−0.0593	1.1053	0.096*
C20	0.21162 (8)	0.4321 (3)	1.11138 (9)	0.0407 (5)
C21	0.26530 (9)	0.4262 (4)	1.15526 (10)	0.0491 (6)
H21	0.2851	0.3512	1.1466	0.059*
C22	0.28909 (10)	0.5325 (4)	1.21193 (11)	0.0603 (7)
H22	0.3252	0.5284	1.2418	0.072*
C23	0.26000 (11)	0.6446 (4)	1.22477 (11)	0.0618 (7)
H23	0.2764	0.7173	1.2630	0.074*
C24	0.20683 (11)	0.6495 (4)	1.18132 (12)	0.0603 (7)
H24	0.1873	0.7256	1.1902	0.072*
C25	0.18209 (9)	0.5423 (3)	1.12451 (11)	0.0493 (6)
H25	0.1459	0.5441	1.0953	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0819 (5)	0.1383 (8)	0.0487 (4)	0.0290 (5)	0.0433 (4)	0.0191 (4)
O1	0.0649 (11)	0.0630 (12)	0.0327 (8)	−0.0080 (9)	0.0249 (8)	0.0011 (8)
O2	0.1223 (16)	0.0849 (15)	0.0484 (10)	−0.0433 (13)	0.0429 (11)	−0.0191 (11)
O3	0.0628 (10)	0.0451 (10)	0.0453 (9)	0.0098 (8)	0.0292 (8)	0.0067 (8)
N1	0.0438 (11)	0.0510 (13)	0.0350 (10)	−0.0041 (9)	0.0196 (9)	0.0035 (9)
N2	0.0558 (12)	0.0353 (11)	0.0403 (11)	0.0024 (9)	0.0264 (9)	0.0060 (9)
N3	0.0486 (11)	0.0378 (11)	0.0362 (10)	0.0034 (9)	0.0227 (9)	0.0037 (9)
C1	0.0691 (17)	0.0617 (18)	0.0473 (15)	−0.0138 (14)	0.0271 (13)	−0.0019 (13)
C2	0.0658 (17)	0.076 (2)	0.0518 (15)	−0.0055 (15)	0.0329 (14)	0.0155 (15)
C3	0.0397 (14)	0.085 (2)	0.0363 (13)	0.0086 (13)	0.0207 (11)	0.0081 (14)
C4	0.0487 (14)	0.0705 (19)	0.0429 (14)	−0.0070 (13)	0.0226 (12)	−0.0091 (13)
C5	0.0493 (14)	0.0601 (17)	0.0431 (14)	−0.0091 (12)	0.0243 (12)	−0.0016 (12)
C6	0.0403 (13)	0.0580 (16)	0.0341 (12)	−0.0036 (12)	0.0164 (11)	0.0032 (12)

C7	0.0552 (15)	0.0600 (17)	0.0389 (14)	−0.0072 (13)	0.0223 (13)	0.0001 (13)
C8	0.0448 (13)	0.0616 (17)	0.0300 (11)	0.0011 (12)	0.0184 (11)	0.0051 (12)
C9	0.0619 (15)	0.0588 (17)	0.0437 (14)	0.0055 (13)	0.0317 (12)	−0.0005 (12)
C10	0.0571 (15)	0.0557 (16)	0.0432 (13)	0.0141 (12)	0.0260 (12)	0.0096 (12)
C11	0.0446 (13)	0.0555 (16)	0.0337 (12)	0.0056 (12)	0.0191 (11)	0.0051 (11)
C12	0.0730 (17)	0.0668 (18)	0.0444 (14)	0.0189 (14)	0.0368 (13)	0.0076 (13)
C13	0.0661 (17)	0.0648 (18)	0.0433 (14)	0.0217 (14)	0.0288 (13)	0.0147 (13)
C14	0.0527 (14)	0.0588 (16)	0.0394 (13)	0.0003 (13)	0.0265 (11)	0.0000 (12)
C15	0.0404 (12)	0.0387 (13)	0.0355 (12)	−0.0043 (10)	0.0209 (10)	0.0016 (10)
C16	0.0432 (13)	0.0396 (14)	0.0432 (13)	−0.0050 (11)	0.0253 (11)	0.0005 (11)
C17	0.0391 (12)	0.0371 (14)	0.0380 (12)	−0.0029 (11)	0.0199 (10)	0.0040 (11)
C18	0.0743 (17)	0.0459 (16)	0.0612 (15)	−0.0013 (13)	0.0442 (14)	0.0006 (12)
C19	0.0869 (19)	0.0444 (16)	0.0569 (15)	0.0035 (14)	0.0406 (14)	0.0147 (13)
C20	0.0519 (14)	0.0370 (13)	0.0339 (12)	−0.0030 (11)	0.0256 (11)	0.0046 (10)
C21	0.0502 (14)	0.0572 (16)	0.0397 (13)	0.0006 (12)	0.0264 (12)	0.0057 (12)
C22	0.0559 (15)	0.0743 (19)	0.0383 (13)	−0.0053 (14)	0.0209 (12)	0.0025 (13)
C23	0.079 (2)	0.0604 (18)	0.0393 (14)	−0.0069 (15)	0.0313 (15)	−0.0047 (12)
C24	0.082 (2)	0.0554 (17)	0.0581 (16)	0.0026 (14)	0.0494 (16)	−0.0023 (14)
C25	0.0543 (14)	0.0489 (15)	0.0480 (13)	−0.0005 (12)	0.0320 (12)	0.0043 (12)

Geometric parameters (Å, °)

Cl1—C3	1.742 (2)	C10—H10	0.9300
O1—C7	1.355 (3)	C11—C12	1.380 (3)
O1—C8	1.408 (2)	C11—C14	1.472 (3)
O2—C7	1.204 (3)	C12—C13	1.389 (3)
O3—C17	1.239 (3)	C12—H12	0.9300
N1—C14	1.280 (3)	C13—H13	0.9300
N1—C15	1.400 (3)	C14—H14	0.9300
N2—C16	1.358 (3)	C15—C16	1.371 (3)
N2—N3	1.400 (2)	C15—C17	1.430 (3)
N2—C19	1.464 (3)	C16—C18	1.484 (3)
N3—C17	1.412 (3)	C18—H18A	0.9600
N3—C20	1.431 (3)	C18—H18B	0.9600
C1—C2	1.379 (3)	C18—H18C	0.9600
C1—C6	1.384 (3)	C19—H19A	0.9600
C1—H1	0.9300	C19—H19B	0.9600
C2—C3	1.375 (4)	C19—H19C	0.9600
C2—H2	0.9300	C20—C21	1.382 (3)
C3—C4	1.366 (3)	C20—C25	1.383 (3)
C4—C5	1.386 (3)	C21—C22	1.375 (3)
C4—H4	0.9300	C21—H21	0.9300
C5—C6	1.380 (3)	C22—C23	1.374 (3)
C5—H5	0.9300	C22—H22	0.9300
C6—C7	1.481 (3)	C23—C24	1.369 (3)
C8—C9	1.368 (3)	C23—H23	0.9300
C8—C13	1.371 (3)	C24—C25	1.379 (3)
C9—C10	1.377 (3)	C24—H24	0.9300
C9—H9	0.9300	C25—H25	0.9300

C10—C11	1.387 (3)		
C7—O1—C8	120.77 (18)	C8—C13—H13	120.9
C14—N1—C15	120.2 (2)	C12—C13—H13	120.9
C16—N2—N3	107.82 (16)	N1—C14—C11	121.7 (2)
C16—N2—C19	125.42 (19)	N1—C14—H14	119.1
N3—N2—C19	118.44 (18)	C11—C14—H14	119.1
N2—N3—C17	108.53 (17)	C16—C15—N1	122.2 (2)
N2—N3—C20	118.83 (16)	C16—C15—C17	108.37 (19)
C17—N3—C20	122.04 (18)	N1—C15—C17	129.3 (2)
C2—C1—C6	121.0 (2)	N2—C16—C15	109.73 (19)
C2—C1—H1	119.5	N2—C16—C18	121.21 (19)
C6—C1—H1	119.5	C15—C16—C18	129.0 (2)
C3—C2—C1	118.5 (2)	O3—C17—N3	122.4 (2)
C3—C2—H2	120.8	O3—C17—C15	132.6 (2)
C1—C2—H2	120.8	N3—C17—C15	105.01 (19)
C4—C3—C2	122.0 (2)	C16—C18—H18A	109.5
C4—C3—Cl1	119.2 (2)	C16—C18—H18B	109.5
C2—C3—Cl1	118.9 (2)	H18A—C18—H18B	109.5
C3—C4—C5	118.9 (2)	C16—C18—H18C	109.5
C3—C4—H4	120.5	H18A—C18—H18C	109.5
C5—C4—H4	120.5	H18B—C18—H18C	109.5
C6—C5—C4	120.5 (2)	N2—C19—H19A	109.5
C6—C5—H5	119.7	N2—C19—H19B	109.5
C4—C5—H5	119.7	H19A—C19—H19B	109.5
C5—C6—C1	119.1 (2)	N2—C19—H19C	109.5
C5—C6—C7	122.5 (2)	H19A—C19—H19C	109.5
C1—C6—C7	118.4 (2)	H19B—C19—H19C	109.5
O2—C7—O1	123.7 (2)	C21—C20—C25	120.4 (2)
O2—C7—C6	124.4 (2)	C21—C20—N3	121.0 (2)
O1—C7—C6	111.9 (2)	C25—C20—N3	118.50 (19)
C9—C8—C13	121.4 (2)	C22—C21—C20	119.3 (2)
C9—C8—O1	115.8 (2)	C22—C21—H21	120.4
C13—C8—O1	122.7 (2)	C20—C21—H21	120.4
C8—C9—C10	119.7 (2)	C23—C22—C21	120.6 (2)
C8—C9—H9	120.1	C23—C22—H22	119.7
C10—C9—H9	120.1	C21—C22—H22	119.7
C9—C10—C11	120.9 (2)	C24—C23—C22	120.0 (2)
C9—C10—H10	119.6	C24—C23—H23	120.0
C11—C10—H10	119.6	C22—C23—H23	120.0
C12—C11—C10	117.8 (2)	C23—C24—C25	120.4 (2)
C12—C11—C14	120.1 (2)	C23—C24—H24	119.8
C10—C11—C14	122.1 (2)	C25—C24—H24	119.8
C11—C12—C13	122.0 (2)	C24—C25—C20	119.3 (2)
C11—C12—H12	119.0	C24—C25—H25	120.4
C13—C12—H12	119.0	C20—C25—H25	120.4
C8—C13—C12	118.1 (2)		
C16—N2—N3—C17	−7.5 (2)	C12—C11—C14—N1	−170.3 (2)
C19—N2—N3—C17	−157.56 (18)	C10—C11—C14—N1	9.0 (3)

C16—N2—N3—C20	−152.92 (18)	C14—N1—C15—C16	178.8 (2)
C19—N2—N3—C20	57.0 (3)	C14—N1—C15—C17	−6.2 (3)
C6—C1—C2—C3	−0.5 (4)	N3—N2—C16—C15	6.8 (2)
C1—C2—C3—C4	0.1 (4)	C19—N2—C16—C15	154.1 (2)
C1—C2—C3—Cl1	−179.20 (19)	N3—N2—C16—C18	−171.50 (19)
C2—C3—C4—C5	0.6 (4)	C19—N2—C16—C18	−24.1 (3)
Cl1—C3—C4—C5	179.97 (17)	N1—C15—C16—N2	172.45 (18)
C3—C4—C5—C6	−1.1 (3)	C17—C15—C16—N2	−3.4 (2)
C4—C5—C6—C1	0.8 (3)	N1—C15—C16—C18	−9.5 (4)
C4—C5—C6—C7	−176.8 (2)	C17—C15—C16—C18	174.7 (2)
C2—C1—C6—C5	0.0 (4)	N2—N3—C17—O3	−172.80 (18)
C2—C1—C6—C7	177.7 (2)	C20—N3—C17—O3	−28.7 (3)
C8—O1—C7—O2	−4.2 (4)	N2—N3—C17—C15	5.3 (2)
C8—O1—C7—C6	173.80 (18)	C20—N3—C17—C15	149.38 (19)
C5—C6—C7—O2	171.5 (3)	C16—C15—C17—O3	176.6 (2)
C1—C6—C7—O2	−6.1 (4)	N1—C15—C17—O3	1.1 (4)
C5—C6—C7—O1	−6.5 (3)	C16—C15—C17—N3	−1.3 (2)
C1—C6—C7—O1	175.9 (2)	N1—C15—C17—N3	−176.73 (19)
C7—O1—C8—C9	−133.6 (2)	N2—N3—C20—C21	29.5 (3)
C7—O1—C8—C13	49.8 (3)	C17—N3—C20—C21	−111.0 (2)
C13—C8—C9—C10	−1.3 (4)	N2—N3—C20—C25	−153.43 (19)
O1—C8—C9—C10	−178.0 (2)	C17—N3—C20—C25	66.0 (3)
C8—C9—C10—C11	0.0 (4)	C25—C20—C21—C22	−0.5 (3)
C9—C10—C11—C12	1.8 (4)	N3—C20—C21—C22	176.4 (2)
C9—C10—C11—C14	−177.5 (2)	C20—C21—C22—C23	−0.5 (4)
C10—C11—C12—C13	−2.3 (4)	C21—C22—C23—C24	0.7 (4)
C14—C11—C12—C13	177.0 (2)	C22—C23—C24—C25	0.0 (4)
C9—C8—C13—C12	0.9 (4)	C23—C24—C25—C20	−1.0 (4)
O1—C8—C13—C12	177.3 (2)	C21—C20—C25—C24	1.3 (3)
C11—C12—C13—C8	1.0 (4)	N3—C20—C25—C24	−175.8 (2)
C15—N1—C14—C11	178.23 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18C···O3^{i}	0.96	2.46	3.405 (3)	169
C19—H19A···O3^{i}	0.96	2.58	3.497 (3)	161
C2—H2···O3^{ii}	0.93	2.53	3.219 (3)	131

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, −*y*+2, *z*−1/2.

Fig. 1

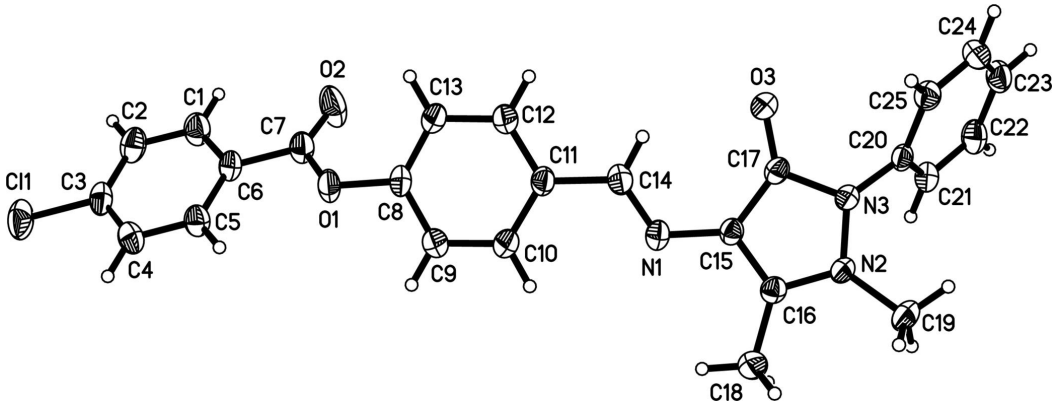
C24
C23
C25
C22
C20
C21
O3
C17
N3
O2
C13
C12
C11
C14
C1
C2
C7
C6
Cl1
C3
C5
O1
C8
C4
C9
C10
N1
C15
N2
C16
C19
C18

Fig. 2