

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(Z)-Ethyl 3-[bis(4-chloro-3-ethyl-1-methyl-1*H*-pyrazol-5-ylcarbonyl)amino]-3-(4-chlorophenyl)-2-cyanopropanoate

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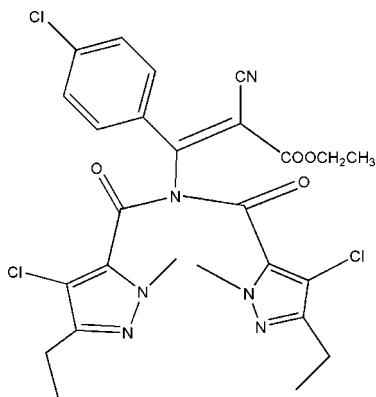
Received 3 December 2008; accepted 11 March 2009

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; disorder in main residue; R factor = 0.065; wR factor = 0.170; data-to-parameter ratio = 14.1.

The title compound, $\text{C}_{26}\text{H}_{25}\text{Cl}_3\text{N}_6\text{O}_4$, was prepared by the reaction of (*Z*)-ethyl 3-amino-3-(4-chlorophenyl)-2-cyanoacrylate and 4-chloro-3-ethyl-1-methyl-1*H*-pyrazole-5-carbonyl chloride. The dihedral angles between the chlorobenzene and the two pyrazole rings are 59.8 (2) and 33.3 (2)°. The two pyrazole rings are oriented to each other at a dihedral angle of 84.7 (2)°. The crystal packing is governed by intermolecular $\text{C}-\text{H}\cdots\text{O}$ interactions, resulting in a three-dimensional network. The ethyl groups are disordered over two positions, with site-occupancy factors of 0.71/0.29 and 0.51/0.49.

Related literature

Several novel acrylate compounds are useful as inhibitors of *Pyricularia oryzae*, *Rhizoctonia solani*, *Botrytis cinerea* and *Gibberella zeae*; see: Heller *et al.* (2004); Creagh & Hubbell (1992); Ibers & Hamilton (1964).



Experimental

Crystal data

$\text{C}_{26}\text{H}_{25}\text{Cl}_3\text{N}_6\text{O}_4$	$V = 2857.21$ (14) Å ³
$M_r = 591.87$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 10.7277$ (3) Å	$\mu = 0.36$ mm ⁻¹
$b = 16.1476$ (5) Å	$T = 298$ K
$c = 17.3109$ (5) Å	$0.20 \times 0.10 \times 0.10$ mm
$\beta = 107.671$ (2)°	

Data collection

Bruker SMART CCD area-detector diffractometer	5600 independent reflections
Absorption correction: none	3595 reflections with $I > 2\sigma(I)$
18010 measured reflections	$R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.065$	12 restraints
$wR(F^2) = 0.170$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.33$ e Å ⁻³
5600 reflections	$\Delta\rho_{\text{min}} = -0.21$ e Å ⁻³
397 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{Cl13}-\text{H13}\cdots\text{O2}^i$	0.93	2.59	3.420 (5)	149

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We thank the Hubei Normal University and the Hunan Provincial Natural Science Fund of China for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2113).

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supporting information

Acta Cryst. (2009). E65, o887 [doi:10.1107/S1600536809008988]

(Z)-Ethyl 3-[bis(4-chloro-3-ethyl-1-methyl-1*H*-pyrazol-5-yl)carbonyl]amino]-3-(4-chlorophenyl)-2-cyanoacrylate

Dehua Zhang, Xiaoyan Zhang and Lijuan Guo

S1. Comment

Recently, 2-cyanoacrylates have been in widespread used as agrochemicals because of their unique mechanism of action and good environmental profiles. The title compound is useful as an inhibitor of *Pyricularia oryzae*, *Rhizoctonia solani*, *Botrytis cinerea* and *Gibberella zeae* (Heller *et al.*, 2004; Ibers & Hamilton, 1964). In the title compound (Fig. 1), all bond lengths and angles are unexceptional. The planar chlorobenzene ring is approximately perpendicular to one of the pyrazole ring with a dihedral angle of 59.9 (2)°. The dihedral angle between this chlorobenzene ring and the other pyrazole rings is 33.3 (12)°. The dihedral angle between the two pyrazole rings is 84.7 (2)°. The crystal packing is governed by C—H...O intermolecular interactions resulting in a three-dimensional network (Table 1.). The ethyl groups are disordered over two positions, with site-occupancy factors of 0.71/0.29 and 0.51/0.49.

S2. Experimental

To a solution of (*Z*)-ethyl 3-amino-3-(4-chlorophenyl)-2-cyanoacrylate (1.25 g, 0.0050 mol) in C₁H₂Cl₂(18 ml), 4-chloro-3-ethyl-1-methyl-1*H*-pyrazole-5-carbonyl chloride (3.11 g, 0.015 mol) was added. Subsequently, Et₃N₁(1.52 g, 0.015 mol) was dropped into the solution under stirring. The reaction mixture was then heated to reflux, stirred for 4 h. Subsequently, it was cooled to room temperature. The reaction solution was filtered off and some white solid was separated. The organic phase was washed with water and then dried over Na₂S₁O₄. After removal of the solvent, a brown dope was obtained. After column chromatogram using ethylacetate/light petroleum (1:6) as the eluent, small single crystals were grown from a solution of ethyl acetate/petroleum ether(3:1) after 45 days, at room temperature.

S3. Refinement

Methyl H atoms were placed in calculated positions with C—H=0.96Å and the torsion angle was refined to fit the electron density; thermal parameters were refined as $U_{\text{iso}}(\text{H})=1.5U_{\text{eq}}(\text{C})$. Other H atoms were placed in calculated positions with C—H =0.96Å (methylene C—H) and 0.93Å (aromatic C—H), and refined in riding mode, with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$.

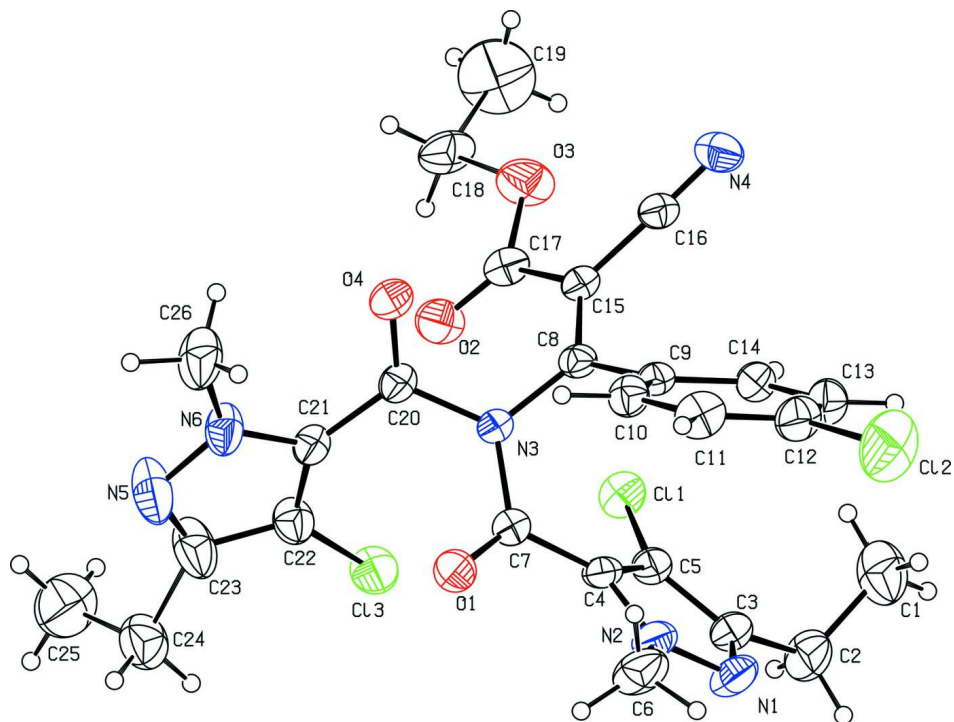
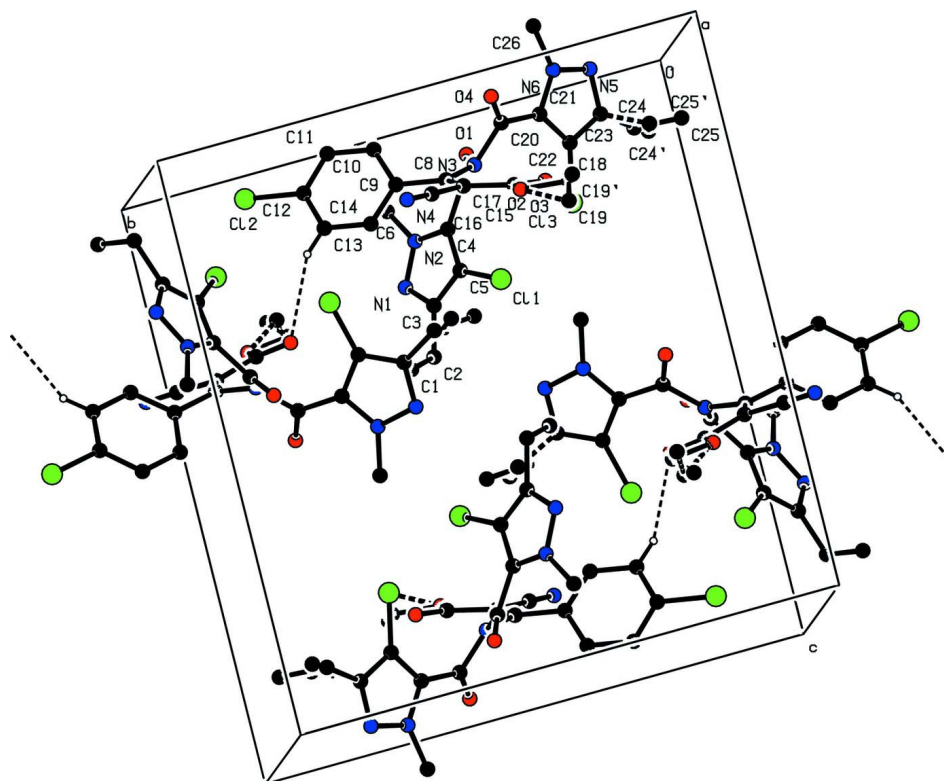


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Only the higher occupied of the disordered sites is shown.

**Figure 2**

The packing of the title compound, viewed down the *c*-axis.

(Z)-Ethyl 3-[bis(4-chloro-3-ethyl-1-methyl-1*H*-pyrazol-5-yl)amino]-3-(4-chlorophenyl)-2-cyanopropanoate

Crystal data

$C_{26}H_{25}Cl_3N_6O_4$

$M_r = 591.87$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 10.7277\ (3)\ \text{\AA}$

$b = 16.1476\ (5)\ \text{\AA}$

$c = 17.3109\ (5)\ \text{\AA}$

$\beta = 107.671\ (2)^\circ$

$V = 2857.21\ (14)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1224$

$D_x = 1.376\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2499 reflections

$\theta = 2.4\text{--}20.2^\circ$

$\mu = 0.36\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Block, colorless

$0.20 \times 0.10 \times 0.10\ \text{mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

18010 measured reflections

5600 independent reflections

3595 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.8^\circ$

$h = -13 \rightarrow 13$

$k = -14 \rightarrow 19$

$l = -19 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.065$
 $wR(F^2) = 0.170$
 $S = 1.02$
 5600 reflections
 397 parameters
 12 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0809P)^2 + 0.6207P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.5605 (5)	1.1026 (3)	0.0809 (3)	0.1016 (16)	
H1A	0.4925	1.0742	0.0957	0.152*	
H1B	0.5308	1.1155	0.0241	0.152*	
H1C	0.5823	1.1529	0.1116	0.152*	
C2	0.6797 (4)	1.0481 (3)	0.0986 (2)	0.0819 (12)	
H2A	0.6586	0.9991	0.0647	0.098*	
H2B	0.7485	1.0777	0.0846	0.098*	
C3	0.7296 (4)	1.0218 (2)	0.1857 (2)	0.0600 (9)	
C4	0.7612 (3)	0.9620 (2)	0.30584 (19)	0.0464 (8)	
C5	0.6770 (3)	0.9653 (2)	0.22757 (19)	0.0493 (8)	
C6	0.9700 (4)	1.0424 (3)	0.3756 (3)	0.0843 (13)	
H6A	0.9397	1.0573	0.4205	0.126*	
H6B	1.0117	1.0893	0.3598	0.126*	
H6C	1.0316	0.9977	0.3913	0.126*	
C7	0.7665 (3)	0.91302 (19)	0.37875 (18)	0.0446 (7)	
C8	0.5482 (3)	0.96134 (19)	0.37330 (17)	0.0416 (7)	
C9	0.6001 (3)	1.0460 (2)	0.39174 (18)	0.0434 (7)	
C10	0.6964 (3)	1.0615 (2)	0.46510 (19)	0.0518 (8)	
H10	0.7256	1.0188	0.5023	0.062*	
C11	0.7483 (4)	1.1396 (3)	0.4827 (2)	0.0675 (10)	
H11	0.8112	1.1505	0.5320	0.081*	
C12	0.7058 (4)	1.2011 (2)	0.4263 (3)	0.0680 (11)	
C13	0.6112 (4)	1.1884 (2)	0.3540 (2)	0.0641 (10)	
H13	0.5830	1.2315	0.3173	0.077*	
C14	0.5585 (3)	1.1101 (2)	0.3366 (2)	0.0508 (8)	

H14	0.4946	1.1003	0.2875	0.061*	
C15	0.4182 (3)	0.9445 (2)	0.34745 (18)	0.0452 (7)	
C16	0.3269 (3)	1.0107 (2)	0.3428 (2)	0.0504 (8)	
C17	0.3619 (3)	0.8606 (3)	0.3228 (2)	0.0543 (9)	
C20	0.6330 (3)	0.8337 (2)	0.44703 (19)	0.0479 (8)	
C21	0.7060 (3)	0.7572 (2)	0.44792 (19)	0.0491 (8)	
C22	0.7445 (4)	0.7138 (2)	0.3903 (2)	0.0604 (9)	
C23	0.8073 (5)	0.6430 (3)	0.4273 (3)	0.0923 (14)	
C18	0.1713 (16)	0.7798 (7)	0.2921 (11)	0.077 (5)	0.51
H18A	0.2076	0.7451	0.2585	0.093*	0.51
H18B	0.1817	0.7522	0.3435	0.093*	0.51
C19	0.0337 (14)	0.7994 (15)	0.2510 (13)	0.159 (9)	0.51
H19A	-0.0021	0.8289	0.2876	0.238*	0.51
H19B	-0.0145	0.7491	0.2343	0.238*	0.51
H19C	0.0275	0.8332	0.2044	0.238*	0.51
C24	0.8921 (8)	0.5836 (4)	0.3948 (5)	0.089 (2)	0.71
H24A	0.8987	0.6030	0.3431	0.107*	0.71
H24B	0.9794	0.5793	0.4327	0.107*	0.71
C25	0.8247 (9)	0.5025 (4)	0.3851 (6)	0.127 (3)	0.71
H25A	0.8184	0.4845	0.4366	0.191*	0.71
H25B	0.8735	0.4626	0.3650	0.191*	0.71
H25C	0.7385	0.5079	0.3474	0.191*	0.71
C26	0.7327 (5)	0.7275 (3)	0.5962 (2)	0.0921 (14)	
H26A	0.6420	0.7356	0.5914	0.138*	
H26B	0.7811	0.7764	0.6186	0.138*	
H26C	0.7660	0.6812	0.6312	0.138*	
C11	0.53576 (9)	0.91015 (6)	0.18601 (5)	0.0620 (3)	
C12	0.77506 (16)	1.29995 (8)	0.44793 (10)	0.1232 (6)	
C13	0.71509 (10)	0.73843 (6)	0.29021 (5)	0.0700 (3)	
N1	0.8404 (3)	1.0541 (2)	0.23522 (19)	0.0693 (9)	
N2	0.8587 (3)	1.01616 (19)	0.30722 (17)	0.0596 (8)	
N3	0.6432 (2)	0.89762 (15)	0.39096 (14)	0.0414 (6)	
N4	0.2531 (3)	1.0622 (2)	0.3401 (2)	0.0723 (9)	
N5	0.8081 (4)	0.6418 (2)	0.5053 (2)	0.0992 (13)	
N6	0.7463 (3)	0.71124 (19)	0.51636 (17)	0.0667 (8)	
O1	0.8667 (2)	0.88843 (15)	0.42578 (14)	0.0596 (6)	
O2	0.4232 (2)	0.79961 (16)	0.31937 (17)	0.0697 (7)	
O3	0.2329 (2)	0.86236 (17)	0.30416 (18)	0.0849 (9)	
O4	0.5658 (2)	0.84529 (16)	0.48997 (14)	0.0683 (7)	
C19'	0.0535 (17)	0.7807 (15)	0.2940 (10)	0.123 (8)	0.49
H19D	0.0884	0.7667	0.3504	0.184*	0.49
H19E	-0.0025	0.7369	0.2658	0.184*	0.49
H19F	0.0041	0.8311	0.2885	0.184*	0.49
C18'	0.160 (2)	0.7920 (11)	0.2596 (11)	0.099 (7)	0.49
H18C	0.1275	0.8040	0.2020	0.119*	0.49
H18D	0.2153	0.7430	0.2675	0.119*	0.49
C24'	0.8165 (13)	0.5613 (7)	0.3901 (10)	0.064 (4)	0.29
H24C	0.7551	0.5582	0.3359	0.077*	0.29

H24D	0.7973	0.5170	0.4226	0.077*	0.29
C25'	0.9573 (15)	0.5544 (12)	0.3871 (14)	0.114 (8)	0.29
H25D	0.9900	0.6086	0.3813	0.171*	0.29
H25E	0.9590	0.5206	0.3418	0.171*	0.29
H25F	1.0110	0.5296	0.4364	0.171*	0.29

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.120 (4)	0.103 (4)	0.069 (3)	0.023 (3)	0.010 (3)	0.017 (3)
C2	0.106 (3)	0.090 (3)	0.058 (2)	0.009 (3)	0.037 (2)	0.017 (2)
C3	0.068 (2)	0.067 (2)	0.053 (2)	0.007 (2)	0.0323 (19)	0.0092 (18)
C4	0.0394 (17)	0.057 (2)	0.0489 (18)	0.0009 (15)	0.0223 (14)	0.0042 (15)
C5	0.0530 (19)	0.054 (2)	0.0459 (18)	0.0040 (16)	0.0219 (15)	0.0022 (15)
C6	0.051 (2)	0.114 (4)	0.085 (3)	-0.023 (2)	0.016 (2)	0.016 (3)
C7	0.0445 (18)	0.0460 (19)	0.0444 (17)	-0.0024 (15)	0.0150 (14)	-0.0006 (14)
C8	0.0415 (17)	0.0505 (19)	0.0354 (15)	0.0011 (14)	0.0156 (13)	0.0014 (13)
C9	0.0433 (17)	0.0491 (19)	0.0426 (17)	0.0016 (14)	0.0202 (14)	0.0013 (15)
C10	0.060 (2)	0.055 (2)	0.0413 (17)	0.0009 (17)	0.0167 (15)	0.0000 (16)
C11	0.072 (2)	0.072 (3)	0.058 (2)	-0.015 (2)	0.0188 (19)	-0.016 (2)
C12	0.081 (3)	0.046 (2)	0.087 (3)	-0.013 (2)	0.041 (2)	-0.014 (2)
C13	0.074 (2)	0.052 (2)	0.070 (2)	0.0044 (19)	0.027 (2)	0.0065 (19)
C14	0.0527 (19)	0.052 (2)	0.0491 (19)	0.0011 (16)	0.0172 (15)	0.0026 (16)
C15	0.0468 (18)	0.0497 (19)	0.0441 (17)	-0.0018 (15)	0.0213 (14)	0.0034 (15)
C16	0.0428 (18)	0.056 (2)	0.056 (2)	-0.0021 (17)	0.0206 (15)	0.0040 (17)
C17	0.049 (2)	0.066 (3)	0.0500 (19)	-0.0080 (18)	0.0183 (15)	-0.0022 (17)
C20	0.0542 (19)	0.049 (2)	0.0430 (17)	-0.0028 (16)	0.0180 (15)	0.0033 (15)
C21	0.056 (2)	0.047 (2)	0.0459 (18)	-0.0028 (16)	0.0180 (15)	0.0041 (15)
C22	0.074 (2)	0.055 (2)	0.052 (2)	0.0086 (18)	0.0182 (18)	0.0001 (17)
C23	0.140 (4)	0.065 (3)	0.074 (3)	0.039 (3)	0.034 (3)	0.001 (2)
C18	0.057 (7)	0.081 (8)	0.099 (11)	-0.032 (6)	0.031 (7)	-0.017 (7)
C19	0.083 (10)	0.159 (17)	0.20 (2)	-0.053 (9)	-0.012 (13)	-0.026 (17)
C24	0.096 (7)	0.066 (5)	0.106 (6)	0.006 (5)	0.030 (6)	-0.002 (4)
C25	0.169 (9)	0.088 (6)	0.144 (8)	-0.016 (6)	0.076 (6)	-0.025 (6)
C26	0.147 (4)	0.079 (3)	0.053 (2)	0.015 (3)	0.034 (3)	0.016 (2)
Cl1	0.0643 (6)	0.0700 (6)	0.0486 (5)	-0.0069 (4)	0.0125 (4)	-0.0022 (4)
Cl2	0.1617 (14)	0.0646 (8)	0.1425 (13)	-0.0441 (8)	0.0452 (10)	-0.0271 (8)
Cl3	0.0878 (7)	0.0770 (7)	0.0490 (5)	0.0122 (5)	0.0263 (5)	-0.0028 (5)
N1	0.068 (2)	0.085 (2)	0.064 (2)	-0.0108 (18)	0.0332 (17)	0.0137 (18)
N2	0.0485 (16)	0.075 (2)	0.0597 (18)	-0.0044 (15)	0.0225 (14)	0.0099 (16)
N3	0.0416 (14)	0.0435 (15)	0.0420 (13)	-0.0004 (12)	0.0172 (11)	0.0034 (12)
N4	0.0542 (19)	0.074 (2)	0.094 (2)	0.0064 (17)	0.0310 (17)	0.0015 (19)
N5	0.154 (4)	0.066 (2)	0.073 (2)	0.041 (2)	0.027 (2)	0.0145 (19)
N6	0.098 (2)	0.0534 (19)	0.0487 (17)	0.0085 (17)	0.0219 (16)	0.0094 (15)
O1	0.0428 (13)	0.0702 (16)	0.0600 (14)	0.0027 (11)	0.0069 (11)	0.0128 (12)
O2	0.0635 (16)	0.0582 (17)	0.0903 (19)	-0.0093 (14)	0.0278 (14)	-0.0143 (14)
O3	0.0497 (15)	0.082 (2)	0.120 (2)	-0.0187 (14)	0.0214 (15)	-0.0215 (18)
O4	0.0842 (17)	0.0763 (18)	0.0597 (15)	0.0154 (14)	0.0445 (14)	0.0172 (13)

C19'	0.134 (18)	0.129 (14)	0.128 (14)	-0.063 (14)	0.072 (12)	-0.039 (12)
C18'	0.074 (10)	0.100 (10)	0.122 (15)	-0.028 (7)	0.027 (10)	-0.012 (10)
C24'	0.067 (10)	0.043 (9)	0.081 (10)	-0.003 (8)	0.020 (9)	-0.007 (8)
C25'	0.097 (15)	0.124 (18)	0.142 (17)	0.032 (13)	0.068 (13)	-0.024 (14)

Geometric parameters (Å, °)

C1—C2	1.505 (6)	C20—C21	1.460 (5)
C1—H1A	0.9600	C21—N6	1.353 (4)
C1—H1B	0.9600	C21—C22	1.381 (5)
C1—H1C	0.9600	C22—C23	1.382 (6)
C2—C3	1.499 (5)	C22—C13	1.710 (4)
C2—H2A	0.9700	C23—N5	1.348 (5)
C2—H2B	0.9700	C23—C24'	1.484 (9)
C3—N1	1.343 (5)	C23—C24	1.542 (7)
C3—C5	1.387 (5)	C18—C19	1.465 (10)
C4—N2	1.358 (4)	C18—O3	1.475 (8)
C4—C5	1.383 (4)	C18—H18A	0.9700
C4—C7	1.476 (4)	C18—H18B	0.9700
C5—C11	1.716 (3)	C19—H19A	0.9600
C6—N2	1.465 (5)	C19—H19B	0.9600
C6—H6A	0.9600	C19—H19C	0.9600
C6—H6B	0.9600	C24—C25	1.481 (7)
C6—H6C	0.9600	C24—H24A	0.9700
C7—O1	1.202 (3)	C24—H24B	0.9700
C7—N3	1.423 (4)	C25—H25A	0.9600
C8—C15	1.356 (4)	C25—H25B	0.9600
C8—N3	1.415 (4)	C25—H25C	0.9600
C8—C9	1.475 (4)	C26—N6	1.457 (5)
C9—C14	1.387 (4)	C26—H26A	0.9600
C9—C10	1.395 (4)	C26—H26B	0.9600
C10—C11	1.376 (5)	C26—H26C	0.9600
C10—H10	0.9300	N1—N2	1.349 (4)
C11—C12	1.370 (6)	N5—N6	1.345 (4)
C11—H11	0.9300	O3—C18'	1.458 (9)
C12—C13	1.367 (5)	C19'—C18'	1.456 (10)
C12—C12	1.752 (4)	C19'—H19D	0.9600
C13—C14	1.379 (5)	C19'—H19E	0.9600
C13—H13	0.9300	C19'—H19F	0.9600
C14—H14	0.9300	C18'—H18C	0.9700
C15—C16	1.436 (5)	C18'—H18D	0.9700
C15—C17	1.491 (5)	C24'—C25'	1.531 (10)
C16—N4	1.139 (4)	C24'—H24C	0.9700
C17—O2	1.196 (4)	C24'—H24D	0.9700
C17—O3	1.323 (4)	C25'—H25D	0.9600
C20—O4	1.197 (4)	C25'—H25E	0.9600
C20—N3	1.444 (4)	C25'—H25F	0.9600

C2—C1—H1A	109.5	C16—C15—C17	116.7 (3)
C2—C1—H1B	109.5	N4—C16—C15	178.5 (4)
H1A—C1—H1B	109.5	O2—C17—O3	123.8 (3)
C2—C1—H1C	109.5	O2—C17—C15	125.5 (3)
H1A—C1—H1C	109.5	O3—C17—C15	110.7 (3)
H1B—C1—H1C	109.5	O4—C20—N3	119.2 (3)
C3—C2—C1	113.1 (3)	O4—C20—C21	123.3 (3)
C3—C2—H2A	109.0	N3—C20—C21	117.5 (3)
C1—C2—H2A	109.0	N6—C21—C22	105.6 (3)
C3—C2—H2B	109.0	N6—C21—C20	120.0 (3)
C1—C2—H2B	109.0	C22—C21—C20	134.3 (3)
H2A—C2—H2B	107.8	C21—C22—C23	107.1 (3)
N1—C3—C5	110.1 (3)	C21—C22—C13	127.6 (3)
N1—C3—C2	120.5 (3)	C22—C21—C20	134.3 (3)
C5—C3—C2	129.4 (4)	C21—C22—C23	107.1 (3)
N2—C4—C5	105.2 (3)	C21—C22—C13	127.6 (3)
N2—C4—C7	120.0 (3)	C23—C22—C13	125.2 (3)
C5—C4—C7	134.7 (3)	N5—C23—C22	109.3 (3)
C4—C5—C3	106.8 (3)	N5—C23—C24'	116.2 (8)
C4—C5—C11	128.4 (3)	C22—C23—C24'	128.4 (8)
C3—C5—C11	124.7 (3)	N5—C23—C24	122.2 (5)
N2—C6—H6A	109.5	C22—C23—C24	127.2 (5)
N2—C6—H6B	109.5	C19—C18—O3	102.4 (8)
H6A—C6—H6B	109.5	C19—C18—H18A	111.3
N2—C6—H6C	109.5	O3—C18—H18A	111.3
H6A—C6—H6C	109.5	C19—C18—H18B	111.3
H6B—C6—H6C	109.5	O3—C18—H18B	111.3
O1—C7—N3	121.5 (3)	H18A—C18—H18B	109.2
O1—C7—C4	123.4 (3)	C25—C24—C23	105.6 (6)
N3—C7—C4	115.1 (3)	C25—C24—H24A	110.6
C15—C8—N3	121.8 (3)	C23—C24—H24A	110.6
C15—C8—C9	122.7 (3)	C25—C24—H24B	110.6
N3—C8—C9	115.3 (2)	C23—C24—H24B	110.6
C14—C9—C10	119.2 (3)	H24A—C24—H24B	108.7
C14—C9—C8	121.5 (3)	N6—C26—H26A	109.5
C10—C9—C8	119.3 (3)	N6—C26—H26B	109.5
C11—C10—C9	120.3 (3)	H26A—C26—H26B	109.5
C11—C10—H10	119.9	N6—C26—H26C	109.5
C9—C10—H10	119.9	H26A—C26—H26C	109.5
C12—C11—C10	118.8 (3)	H26B—C26—H26C	109.5
C12—C11—H11	120.6	C3—N1—N2	105.4 (3)
C10—C11—H11	120.6	N1—N2—C4	112.4 (3)
C13—C12—C11	122.5 (3)	N1—N2—C6	118.0 (3)
C13—C12—C12	118.8 (3)	C4—N2—C6	129.4 (3)
C11—C12—C12	118.7 (3)	C8—N3—C7	118.8 (2)
C12—C13—C14	118.6 (4)	C8—N3—C20	117.9 (2)
C12—C13—H13	120.7	C7—N3—C20	119.2 (2)
C14—C13—H13	120.7	N6—N5—C23	106.1 (3)

C13—C14—C9	120.6 (3)	N5—N6—C21	111.9 (3)
C13—C14—H14	119.7	N5—N6—C26	118.7 (3)
C9—C14—H14	119.7	C21—N6—C26	129.4 (3)
C8—C15—C16	119.0 (3)	C17—O3—C18'	117.5 (10)
C8—C15—C17	124.3 (3)	C17—O3—C18	114.0 (8)
C16—C15—C17	116.7 (3)	C18'—C19'—H19D	109.5
N4—C16—C15	178.5 (4)	C18'—C19'—H19E	109.5
O2—C17—O3	123.8 (3)	H19D—C19'—H19E	109.5
O2—C17—C15	125.5 (3)	C18'—C19'—H19F	109.5
O3—C17—C15	110.7 (3)	H19D—C19'—H19F	109.5
O4—C20—N3	119.2 (3)	H19E—C19'—H19F	109.5
O4—C20—C21	123.3 (3)	C19'—C18'—O3	103.9 (9)
N3—C20—C21	117.5 (3)	C19'—C18'—H18C	111.0
N6—C21—C22	105.6 (3)	O3—C18'—H18C	111.0
N6—C21—C20	120.0 (3)	C19'—C18'—H18D	111.0
C22—C21—C20	134.3 (3)	O3—C18'—H18D	111.0
C21—C22—C23	107.1 (3)	H18C—C18'—H18D	109.0
C21—C22—C13	127.6 (3)	C23—C24'—C25'	106.0 (8)
C10—C11—H11	120.6	C23—C24'—H24C	110.5
C13—C12—C11	122.5 (3)	C25'—C24'—H24C	110.5
C13—C12—C12	118.8 (3)	C23—C24'—H24D	110.5
C11—C12—C12	118.7 (3)	C25'—C24'—H24D	110.5
C12—C13—C14	118.6 (4)	H24C—C24'—H24D	108.7
C12—C13—H13	120.7	C24'—C25'—H25D	109.5
C14—C13—H13	120.7	C24'—C25'—H25E	109.5
C13—C14—C9	120.6 (3)	H25D—C25'—H25E	109.5
C13—C14—H14	119.7	C24'—C25'—H25F	109.5
C9—C14—H14	119.7	H25D—C25'—H25F	109.5
C8—C15—C16	119.0 (3)	H25E—C25'—H25F	109.5
C8—C15—C17	124.3 (3)		
C1—C2—C3—N1	-107.3 (5)	C13—C22—C23—C24'	-26.2 (10)
C1—C2—C3—C5	72.6 (6)	C21—C22—C23—C24	-166.6 (5)
N2—C4—C5—C3	0.2 (4)	C13—C22—C23—C24	16.2 (8)
C7—C4—C5—C3	-176.8 (3)	N5—C23—C24—C25	76.6 (8)
N2—C4—C5—C11	178.8 (2)	C22—C23—C24—C25	-118.3 (7)
C7—C4—C5—C11	1.8 (6)	C24'—C23—C24—C25	-12.9 (14)
N1—C3—C5—C4	-1.2 (4)	C5—C3—N1—N2	1.6 (4)
C2—C3—C5—C4	178.9 (4)	C2—C3—N1—N2	-178.4 (3)
N1—C3—C5—C11	-179.8 (3)	C3—N1—N2—C4	-1.6 (4)
C2—C3—C5—C11	0.2 (6)	C3—N1—N2—C6	-176.7 (3)
N2—C4—C7—O1	-33.8 (5)	C5—C4—N2—N1	0.8 (4)
C5—C4—C7—O1	142.9 (4)	C7—C4—N2—N1	178.4 (3)
N2—C4—C7—N3	145.1 (3)	C5—C4—N2—C6	175.3 (4)
C5—C4—C7—N3	-38.2 (5)	C7—C4—N2—C6	-7.1 (5)
C15—C8—C9—C14	-51.9 (4)	C15—C8—N3—C7	149.4 (3)
N3—C8—C9—C14	133.3 (3)	C9—C8—N3—C7	-35.7 (4)
C15—C8—C9—C10	130.3 (3)	C15—C8—N3—C20	-53.3 (4)

N3—C8—C9—C10	-44.5 (4)	C9—C8—N3—C20	121.6 (3)
C14—C9—C10—C11	0.7 (5)	O1—C7—N3—C8	140.0 (3)
C8—C9—C10—C11	178.5 (3)	C4—C7—N3—C8	-38.9 (4)
C9—C10—C11—C12	-1.4 (5)	O1—C7—N3—C20	-17.0 (4)
C10—C11—C12—C13	1.7 (6)	C4—C7—N3—C20	164.1 (3)
C10—C11—C12—C12	-178.5 (3)	O4—C20—N3—C8	-16.6 (4)
C11—C12—C13—C14	-1.3 (6)	C21—C20—N3—C8	163.2 (3)
C12—C12—C13—C14	178.9 (3)	O4—C20—N3—C7	140.6 (3)
C12—C13—C14—C9	0.5 (5)	C21—C20—N3—C7	-39.6 (4)
C10—C9—C14—C13	-0.2 (5)	C22—C23—N5—N6	0.0 (6)
C8—C9—C14—C13	-178.0 (3)	C24'—C23—N5—N6	-154.8 (7)
N3—C8—C15—C16	170.3 (3)	C24—C23—N5—N6	167.5 (5)
C9—C8—C15—C16	-4.3 (4)	C23—N5—N6—C21	-0.2 (5)
N3—C8—C15—C17	-9.9 (5)	C23—N5—N6—C26	-179.5 (4)
C9—C8—C15—C17	175.6 (3)	C22—C21—N6—N5	0.2 (4)
C8—C15—C17—O2	-3.5 (5)	C20—C21—N6—N5	178.0 (3)
C16—C15—C17—O2	176.4 (3)	C22—C21—N6—C26	179.5 (4)
C8—C15—C17—O3	177.0 (3)	C20—C21—N6—C26	-2.8 (6)
C16—C15—C17—O3	-3.1 (4)	O2—C17—O3—C18'	-14.9 (10)
O4—C20—C21—N6	-27.8 (5)	C15—C17—O3—C18'	164.7 (9)
N3—C20—C21—N6	152.4 (3)	O2—C17—O3—C18	9.9 (9)
O4—C20—C21—C22	149.1 (4)	C15—C17—O3—C18	-170.5 (8)
N3—C20—C21—C22	-30.7 (5)	C19—C18—O3—C17	-164.7 (12)
N6—C21—C22—C23	-0.2 (4)	C19—C18—O3—C18'	-60 (4)
C20—C21—C22—C23	-177.4 (4)	C17—O3—C18'—C19'	142.5 (12)
N6—C21—C22—C13	176.9 (3)	C18—O3—C18'—C19'	56 (4)
C20—C21—C22—C13	-0.3 (6)	N5—C23—C24'—C25'	-103.8 (14)
C21—C22—C23—N5	0.1 (6)	C22—C23—C24'—C25'	107.0 (14)
C13—C22—C23—N5	-177.1 (3)	C24—C23—C24'—C25'	5.7 (12)
C21—C22—C23—C24'	151.0 (8)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C13—H13 \cdots O2 ⁱ	0.93	2.59	3.420 (5)	149

Symmetry code: (i) $-x+1, y+1/2, -z+1/2$.