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N-{2-Chloro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)-1,2,3,6-tetrahydropyrimidinyl]phenyl}-2,2-bis(3-fluorophenoxy)acetamide

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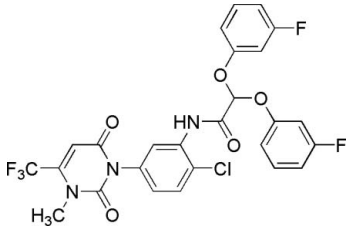
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.054; wR factor = 0.163; data-to-parameter ratio = 14.8.

The title compound, $C_{26}H_{17}ClF_5N_3O_5$, belongs to a new class of amide compounds having potential biological activity. The pyrimidine ring makes a dihedral angle of 61.66 (2)° with the adjacent benzene ring. The dihedral angle between the other two benzene rings is 73.12 (1)°. There are intramolecular C—H···O, C—H···F, N—H···O and N—H···Cl hydrogen bonds. One of the fluorophenyl groups is disordered over two positions in a ratio of *ca.* 3:1. The molecules are connected by intermolecular Cl···O non-bonded interactions [Cl···O = 3.054 (2) Å], forming a dimer.

Related literature

For the preparation of the title compound, see: Huang *et al.* (2006). For related literature, see: Bruno *et al.* (1997).



Experimental

Crystal data

$C_{26}H_{17}ClF_5N_3O_5$
M_r = 581.88
Monoclinic, $P2_1/n$
a = 16.2280 (13) Å
b = 6.7102 (6) Å
c = 23.772 (2) Å
β = 100.5880 (10)°
V = 2544.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 299 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick,1997)
T_{min} = 0.934, T_{max} = 0.955
22744 measured reflections
5563 independent reflections
4336 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.163
S = 1.03
5563 reflections
375 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O3	0.93	2.31	2.896 (3)	121
C6—H6*C*···F2	0.96	2.37	3.046 (4)	127
N3—H3*A*···O5	0.85 (4)	2.07 (4)	2.545 (2)	115 (3)
N3—H3*A*···Cl1	0.85 (4)	2.44 (4)	2.9074 (19)	115 (3)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

The author is grateful to Xiangfan University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2230).

References

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Bruno, I. J., Cole, J. C., Lommerse, J. P. M., Rowland, R. S., Taylor, R. & Verdonk, M. L. (1997). *J. Comput. Mol. Des.* **11**, 525–537.
Huang, M.-Z., Zhang, Q., Ren, Y.-G., Lei, M.-X., Huang, L., Ren, J. & Yang, G.-F. (2006). *Youji Huaxue* (*Chin. J. Org. Chem.*) **26**, 1539–1543.
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supplementary materials

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N-{2-Chloro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)-1,2,3,6-tetrahydropyrimidinyl]phenyl}-2,2-bis(3-fluorophenoxy)acetamide

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Comment

The title compound, (I), is a new class of amide compounds having potential biological activity. Preliminary bioassay showed that the title compound had good herbicidal activity (Huang *et al.*, 2006).

The molecular structure of (I) is shown in Fig. 1. The torsion angle of C9—N3—C14—C15 is 179.1 (2)°. The molecules are connected by two intermolecular Cl···O nonbonded interactions (Bruno *et al.*, 1997) to form a dimer. The distance between atom Cl1 and atom O1 at (2 − *x*, 1 − *y*, 2 − *z*) is 3.0542 (18) Å. The crystal packing is stabilized by van der Waals forces.

Experimental

The title compound was synthesized according to the procedure of Huang *et al.* (2006) in 85% isolated yield. Crystals of (I) suitable for X-ray data collection were obtained by slow evaporation of a DMF and MeOH solution in a ratio of 4:1 at 293 K.

Refinement

One of the fluorophenyl groups was found to be disordered over two orientations. The occupancies refined to 0.751 (5) and 0.249 (5). The N-bound H atom was located in a difference map and the positional parameters were refined, with U_{iso}(H) = 1.2U_{eq}(N). The refined N—H distance is 0.85 (4) Å. Other H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

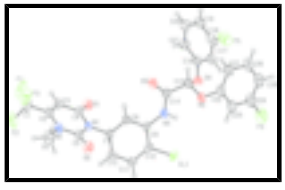

Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by spheres of arbitrary radius. Only one component of the disordered fluorophenyl group is shown.

N-{2-Chloro-5-[3-methyl-2,6-dioxo-4-(trifluoromethyl)-1,2,3,6- tetrahydropyrimidinyl]phenyl}-2,2-bis(3-fluorophenoxy)acetamide

Crystal data

$C_{26}H_{17}ClF_5N_3O_5$	F_{000} = 1184
M_r = 581.88	D_x = 1.519 Mg m^{-3}

Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 7373 reflections
$a = 16.2280\ (13)$ Å	$\theta = 2.6–26.7°$
$b = 6.7102\ (6)$ Å	$\mu = 0.23$ mm^{-1}
$c = 23.772\ (2)$ Å	$T = 299\ (2)$ K
$\beta = 100.5880\ (10)°$	Block, colorless
$V = 2544.5\ (4)$ Å^3	0.30 × 0.20 × 0.20 mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area detector diffractometer	5563 independent reflections
Radiation source: fine-focus sealed tube	4336 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 299(2)$ K	$\theta_{max} = 27.0°$
φ and ω scans	$\theta_{min} = 1.7°$
Absorption correction: multi-scan (*SADABS*; Sheldrick,1997)	$h = -20\rightarrow20$
$T_{min} = 0.934$, $T_{max} = 0.955$	$k = -8\rightarrow8$
22744 measured reflections	$l = -30\rightarrow30$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.163$	$w = 1/[\sigma^2(F_o^2) + (0.0929P)^2 + 0.7196P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
5563 reflections	$\Delta\rho_{max} = 0.47$ e Å^{-3}
375 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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}	Occ. (<1)
C1	0.88345 (19)	0.9362 (5)	0.64714 (12)	0.0825 (8)	
C2	0.88883 (14)	0.8305 (3)	0.70435 (9)	0.0552 (5)	
C3	0.93968 (15)	0.9015 (3)	0.74941 (9)	0.0588 (5)	
H3	0.9698	1.0172	0.7458	0.071*	
C4	0.94969 (14)	0.8034 (3)	0.80437 (9)	0.0506 (5)	
C5	0.84156 (14)	0.5638 (3)	0.75695 (9)	0.0534 (5)	
C6	0.7834 (2)	0.5816 (5)	0.65599 (11)	0.0881 (9)	
H6A	0.7297	0.6451	0.6529	0.132*	
H6B	0.7772	0.4408	0.6610	0.132*	
H6C	0.8053	0.6057	0.6218	0.132*	
C7	0.90085 (12)	0.5314 (3)	0.85767 (8)	0.0455 (4)	
C8	0.87154 (12)	0.6237 (3)	0.90172 (8)	0.0454 (4)	
H8	0.8468	0.7489	0.8964	0.055*	
C9	0.87921 (12)	0.5283 (3)	0.95440 (8)	0.0440 (4)	
C10	0.91616 (12)	0.3399 (3)	0.96041 (8)	0.0454 (4)	
C11	0.94398 (14)	0.2474 (3)	0.91578 (9)	0.0524 (5)	
H11	0.9674	0.1207	0.9205	0.063*	
C12	0.93680 (14)	0.3443 (3)	0.86379 (9)	0.0519 (5)	
H12	0.9559	0.2843	0.8333	0.062*	
C14	0.80870 (14)	0.7796 (3)	1.00481 (9)	0.0538 (5)	
C15	0.79113 (15)	0.8288 (4)	1.06480 (9)	0.0568 (5)	
H15	0.8123	0.9617	1.0770	0.068*	
C16	0.65624 (14)	0.9874 (3)	1.05906 (8)	0.0529 (5)	
C17	0.57840 (15)	0.9618 (4)	1.07377 (10)	0.0651 (6)	
H17	0.5623	0.8388	1.0862	0.078*	
C18	0.52584 (16)	1.1224 (5)	1.06957 (12)	0.0747 (7)	
H18	0.4729	1.1055	1.0786	0.090*	0.249 (5)
C19	0.5473 (2)	1.3048 (5)	1.05286 (12)	0.0805 (8)	
H19	0.5111	1.4128	1.0518	0.097*	
C20	0.6237 (2)	1.3247 (4)	1.03773 (13)	0.0836 (8)	
H20	0.6391	1.4482	1.0252	0.100*	0.751 (5)
C21	0.67913 (18)	1.1675 (4)	1.04039 (12)	0.0715 (7)	
H21	0.7310	1.1842	1.0297	0.086*	
C22	0.83759 (15)	0.7165 (4)	1.16139 (9)	0.0615 (6)	
C23	0.87687 (17)	0.5641 (5)	1.19444 (10)	0.0733 (7)	
H23	0.8940	0.4497	1.1777	0.088*	
C24	0.8901 (2)	0.5852 (5)	1.25253 (11)	0.0857 (9)	
C25	0.8651 (2)	0.7482 (5)	1.27896 (12)	0.0861 (9)	
H25	0.8746	0.7573	1.3187	0.103*	
C26	0.82576 (19)	0.8982 (5)	1.24552 (12)	0.0824 (8)	
H26	0.8086	1.0118	1.2626	0.099*	
C27	0.81105 (19)	0.8823 (5)	1.18607 (11)	0.0767 (8)	

H27	0.7834	0.9838	1.1634	0.092*	
Cl1	0.93109 (4)	0.22525 (8)	1.02710 (2)	0.05918 (19)	
F1	0.93072 (17)	1.1027 (4)	0.65464 (9)	0.1384 (9)	
F2	0.91365 (15)	0.8294 (4)	0.60997 (7)	0.1204 (8)	
F3	0.80970 (13)	0.9976 (4)	0.62507 (9)	0.1256 (8)	
F4	0.92954 (19)	0.4374 (4)	1.28489 (8)	0.1533 (11)	
F5	0.44825 (14)	1.0954 (5)	1.08063 (13)	0.1160 (12)	0.751 (5)
F5'	0.6391 (6)	1.4752 (10)	1.0068 (3)	0.107 (3)	0.249 (5)
H3A	0.871 (2)	0.556 (6)	1.0340 (17)	0.129*	
N1	0.89657 (11)	0.6373 (2)	0.80425 (6)	0.0469 (4)	
N2	0.84131 (12)	0.6632 (3)	0.70551 (7)	0.0563 (5)	
N3	0.85381 (12)	0.6140 (3)	1.00225 (7)	0.0545 (5)	
O1	0.99850 (12)	0.8528 (3)	0.84664 (7)	0.0683 (5)	
O2	0.79781 (12)	0.4212 (3)	0.76047 (7)	0.0780 (5)	
O3	0.78186 (14)	0.8891 (3)	0.96539 (7)	0.0821 (6)	
O4	0.70443 (11)	0.8169 (2)	1.06338 (8)	0.0644 (4)	
O5	0.82930 (12)	0.6831 (3)	1.10315 (6)	0.0727 (5)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0791 (18)	0.114 (2)	0.0576 (15)	0.0048 (17)	0.0198 (14)	0.0289 (15)
C2	0.0572 (13)	0.0653 (13)	0.0473 (11)	0.0154 (10)	0.0206 (10)	0.0139 (9)
C3	0.0713 (14)	0.0582 (12)	0.0500 (12)	0.0016 (11)	0.0192 (11)	0.0115 (9)
C4	0.0623 (13)	0.0472 (10)	0.0445 (10)	0.0022 (9)	0.0158 (9)	0.0032 (8)
C5	0.0579 (12)	0.0604 (12)	0.0425 (10)	0.0002 (10)	0.0109 (9)	0.0020 (9)
C6	0.095 (2)	0.111 (2)	0.0495 (13)	−0.0142 (18)	−0.0110 (13)	−0.0026 (14)
C7	0.0502 (11)	0.0483 (10)	0.0380 (9)	−0.0019 (8)	0.0083 (8)	0.0051 (8)
C8	0.0486 (11)	0.0462 (10)	0.0416 (10)	0.0048 (8)	0.0087 (8)	0.0058 (8)
C9	0.0434 (10)	0.0499 (10)	0.0388 (9)	0.0009 (8)	0.0082 (8)	0.0047 (8)
C10	0.0461 (10)	0.0482 (10)	0.0404 (9)	−0.0019 (8)	0.0037 (8)	0.0115 (8)
C11	0.0602 (13)	0.0432 (10)	0.0532 (11)	0.0066 (9)	0.0088 (10)	0.0064 (8)
C12	0.0624 (13)	0.0499 (11)	0.0448 (10)	0.0037 (9)	0.0135 (9)	0.0000 (8)
C14	0.0592 (13)	0.0590 (12)	0.0436 (10)	0.0067 (10)	0.0104 (9)	0.0033 (9)
C15	0.0629 (13)	0.0612 (12)	0.0482 (11)	0.0120 (10)	0.0156 (10)	0.0051 (9)
C16	0.0584 (12)	0.0557 (12)	0.0454 (10)	0.0053 (10)	0.0119 (9)	−0.0046 (9)
C17	0.0677 (15)	0.0713 (15)	0.0595 (13)	−0.0063 (12)	0.0201 (11)	−0.0160 (11)
C18	0.0584 (15)	0.101 (2)	0.0655 (15)	0.0096 (14)	0.0146 (12)	−0.0249 (14)
C19	0.086 (2)	0.088 (2)	0.0665 (16)	0.0330 (16)	0.0116 (14)	−0.0071 (14)
C20	0.104 (2)	0.0643 (16)	0.0851 (19)	0.0186 (15)	0.0228 (17)	0.0117 (14)
C21	0.0702 (16)	0.0648 (14)	0.0845 (17)	0.0095 (12)	0.0273 (14)	0.0109 (13)
C22	0.0621 (14)	0.0810 (15)	0.0451 (11)	0.0121 (12)	0.0194 (10)	0.0060 (10)
C23	0.0777 (17)	0.0929 (18)	0.0534 (13)	0.0225 (15)	0.0226 (12)	0.0106 (12)
C24	0.0880 (19)	0.117 (2)	0.0524 (14)	0.0277 (18)	0.0141 (13)	0.0201 (15)
C25	0.086 (2)	0.125 (3)	0.0460 (13)	0.0088 (18)	0.0090 (13)	0.0008 (15)
C26	0.090 (2)	0.102 (2)	0.0570 (14)	0.0049 (17)	0.0183 (14)	−0.0113 (14)
C27	0.093 (2)	0.0870 (18)	0.0519 (13)	0.0207 (15)	0.0182 (13)	0.0032 (12)
Cl1	0.0670 (4)	0.0602 (3)	0.0492 (3)	0.0042 (2)	0.0075 (2)	0.0205 (2)

F1	0.168 (2)	0.155 (2)	0.0876 (13)	−0.0499 (18)	0.0122 (13)	0.0612 (14)
F2	0.1407 (18)	0.177 (2)	0.0551 (9)	0.0265 (15)	0.0492 (11)	0.0164 (11)
F3	0.0993 (13)	0.177 (2)	0.0969 (13)	0.0403 (14)	0.0087 (11)	0.0773 (14)
F4	0.210 (3)	0.177 (2)	0.0691 (11)	0.096 (2)	0.0160 (14)	0.0350 (13)
F5	0.0706 (16)	0.134 (2)	0.152 (3)	0.0061 (14)	0.0437 (16)	−0.0359 (19)
F5'	0.156 (8)	0.066 (4)	0.093 (5)	0.022 (4)	0.007 (5)	0.001 (4)
N1	0.0576 (10)	0.0485 (9)	0.0354 (8)	0.0017 (7)	0.0106 (7)	0.0029 (6)
N2	0.0582 (11)	0.0739 (12)	0.0360 (8)	0.0076 (9)	0.0061 (7)	0.0006 (8)
N3	0.0632 (11)	0.0629 (11)	0.0395 (9)	0.0129 (9)	0.0152 (8)	0.0097 (7)
O1	0.0873 (12)	0.0661 (10)	0.0489 (9)	−0.0207 (9)	0.0056 (8)	−0.0010 (7)
O2	0.0875 (12)	0.0848 (12)	0.0570 (10)	−0.0268 (11)	0.0004 (9)	0.0027 (8)
O3	0.1186 (15)	0.0829 (12)	0.0449 (8)	0.0448 (11)	0.0155 (9)	0.0115 (8)
O4	0.0674 (10)	0.0515 (8)	0.0794 (11)	0.0045 (7)	0.0274 (8)	0.0028 (8)
O5	0.0974 (13)	0.0815 (11)	0.0427 (8)	0.0353 (10)	0.0218 (8)	0.0094 (8)

Geometric parameters (Å, °)

C1—F3	1.283 (3)	C14—C15	1.541 (3)
C1—F2	1.302 (4)	C15—O5	1.401 (3)
C1—F1	1.348 (4)	C15—O4	1.403 (3)
C1—C2	1.522 (3)	C15—H15	0.9800
C2—C3	1.315 (3)	C16—C21	1.362 (3)
C2—N2	1.365 (3)	C16—O4	1.379 (3)
C3—C4	1.445 (3)	C16—C17	1.382 (3)
C3—H3	0.9300	C17—C18	1.366 (4)
C4—O1	1.206 (3)	C17—H17	0.9300
C4—N1	1.408 (3)	C18—F5	1.345 (4)
C5—O2	1.204 (3)	C18—C19	1.352 (4)
C5—N1	1.391 (3)	C18—H18	0.9300
C5—N2	1.392 (3)	C19—C20	1.360 (4)
C6—N2	1.471 (3)	C19—H19	0.9300
C6—H6A	0.9600	C20—F5'	1.299 (8)
C6—H6B	0.9600	C20—C21	1.380 (4)
C6—H6C	0.9600	C20—H20	0.9300
C7—C8	1.375 (3)	C21—H21	0.9300
C7—C12	1.380 (3)	C22—C27	1.364 (4)
C7—N1	1.446 (2)	C22—C23	1.373 (3)
C8—C9	1.392 (2)	C22—O5	1.384 (3)
C8—H8	0.9300	C23—C24	1.366 (4)
C9—C10	1.395 (3)	C23—H23	0.9300
C9—N3	1.402 (2)	C24—F4	1.343 (3)
C10—C11	1.375 (3)	C24—C25	1.360 (4)
C10—Cl1	1.7387 (18)	C25—C26	1.366 (4)
C11—C12	1.382 (3)	C25—H25	0.9300
C11—H11	0.9300	C26—C27	1.394 (4)
C12—H12	0.9300	C26—H26	0.9300
C14—O3	1.208 (3)	C27—H27	0.9300
C14—N3	1.338 (3)	N3—H3A	0.85 (4)
F3—C1—F2	109.8 (3)	C21—C16—O4	125.1 (2)

F3—C1—F1	104.7 (3)	C21—C16—C17	120.6 (2)
F2—C1—F1	105.7 (3)	O4—C16—C17	114.2 (2)
F3—C1—C2	114.3 (2)	C18—C17—C16	118.1 (3)
F2—C1—C2	112.5 (3)	C18—C17—H17	121.0
F1—C1—C2	109.3 (2)	C16—C17—H17	121.0
C3—C2—N2	123.61 (19)	F5—C18—C19	118.7 (3)
C3—C2—C1	118.9 (2)	F5—C18—C17	118.3 (3)
N2—C2—C1	117.5 (2)	C19—C18—C17	123.0 (3)
C2—C3—C4	121.4 (2)	C19—C18—H18	118.5
C2—C3—H3	119.3	C17—C18—H18	118.5
C4—C3—H3	119.3	C18—C19—C20	117.6 (3)
O1—C4—N1	121.80 (18)	C18—C19—H19	121.2
O1—C4—C3	125.2 (2)	C20—C19—H19	121.2
N1—C4—C3	113.04 (19)	F5'—C20—C19	120.4 (5)
O2—C5—N1	121.66 (19)	F5'—C20—C21	115.4 (5)
O2—C5—N2	122.4 (2)	C19—C20—C21	122.1 (3)
N1—C5—N2	115.97 (19)	C19—C20—H20	119.0
N2—C6—H6A	109.5	C21—C20—H20	119.0
N2—C6—H6B	109.5	C16—C21—C20	118.6 (3)
H6A—C6—H6B	109.5	C16—C21—H21	120.7
N2—C6—H6C	109.5	C20—C21—H21	120.7
H6A—C6—H6C	109.5	C27—C22—C23	120.8 (2)
H6B—C6—H6C	109.5	C27—C22—O5	125.6 (2)
C8—C7—C12	121.87 (17)	C23—C22—O5	113.7 (2)
C8—C7—N1	118.68 (17)	C24—C23—C22	118.1 (3)
C12—C7—N1	119.40 (17)	C24—C23—H23	120.9
C7—C8—C9	119.47 (18)	C22—C23—H23	120.9
C7—C8—H8	120.3	F4—C24—C25	118.7 (3)
C9—C8—H8	120.3	F4—C24—C23	118.2 (3)
C8—C9—C10	118.33 (17)	C25—C24—C23	123.1 (3)
C8—C9—N3	123.38 (18)	C24—C25—C26	118.1 (3)
C10—C9—N3	118.27 (16)	C24—C25—H25	120.9
C11—C10—C9	121.73 (17)	C26—C25—H25	120.9
C11—C10—Cl1	119.57 (15)	C25—C26—C27	120.6 (3)
C9—C10—Cl1	118.64 (15)	C25—C26—H26	119.7
C10—C11—C12	119.46 (18)	C27—C26—H26	119.7
C10—C11—H11	120.3	C22—C27—C26	119.3 (3)
C12—C11—H11	120.3	C22—C27—H27	120.3
C7—C12—C11	119.11 (19)	C26—C27—H27	120.3
C7—C12—H12	120.4	C5—N1—C4	125.71 (17)
C11—C12—H12	120.4	C5—N1—C7	117.09 (17)
O3—C14—N3	126.3 (2)	C4—N1—C7	117.18 (16)
O3—C14—C15	119.10 (19)	C2—N2—C5	120.07 (18)
N3—C14—C15	114.58 (18)	C2—N2—C6	124.8 (2)
O5—C15—O4	107.31 (18)	C5—N2—C6	115.0 (2)
O5—C15—C14	108.54 (17)	C14—N3—C9	128.49 (17)
O4—C15—C14	108.71 (19)	C14—N3—H3A	115 (3)
O5—C15—H15	110.7	C9—N3—H3A	116 (3)
O4—C15—H15	110.7	C16—O4—C15	120.45 (18)

C14—C15—H15	110.7	C22—O5—C15	119.20 (18)
F3—C1—C2—C3	−121.5 (3)	C22—C23—C24—F4	−179.1 (3)
F2—C1—C2—C3	112.5 (3)	C22—C23—C24—C25	1.1 (5)
F1—C1—C2—C3	−4.6 (4)	F4—C24—C25—C26	179.4 (3)
F3—C1—C2—N2	59.9 (4)	C23—C24—C25—C26	−0.7 (5)
F2—C1—C2—N2	−66.1 (3)	C24—C25—C26—C27	0.7 (5)
F1—C1—C2—N2	176.8 (2)	C23—C22—C27—C26	1.4 (4)
N2—C2—C3—C4	0.8 (4)	O5—C22—C27—C26	−178.2 (3)
C1—C2—C3—C4	−177.7 (2)	C25—C26—C27—C22	−1.0 (5)
C2—C3—C4—O1	175.5 (2)	O2—C5—N1—C4	−179.6 (2)
C2—C3—C4—N1	−3.6 (3)	N2—C5—N1—C4	1.3 (3)
C12—C7—C8—C9	1.0 (3)	O2—C5—N1—C7	1.8 (3)
N1—C7—C8—C9	−176.61 (18)	N2—C5—N1—C7	−177.28 (17)
C7—C8—C9—C10	−0.5 (3)	O1—C4—N1—C5	−176.6 (2)
C7—C8—C9—N3	177.68 (19)	C3—C4—N1—C5	2.6 (3)
C8—C9—C10—C11	−0.6 (3)	O1—C4—N1—C7	2.0 (3)
N3—C9—C10—C11	−178.9 (2)	C3—C4—N1—C7	−178.86 (17)
C8—C9—C10—Cl1	176.62 (15)	C8—C7—N1—C5	−112.3 (2)
N3—C9—C10—Cl1	−1.7 (3)	C12—C7—N1—C5	70.0 (3)
C9—C10—C11—C12	1.3 (3)	C8—C7—N1—C4	69.0 (2)
Cl1—C10—C11—C12	−175.96 (17)	C12—C7—N1—C4	−108.7 (2)
C8—C7—C12—C11	−0.4 (3)	C3—C2—N2—C5	3.5 (3)
N1—C7—C12—C11	177.22 (19)	C1—C2—N2—C5	−177.9 (2)
C10—C11—C12—C7	−0.7 (3)	C3—C2—N2—C6	179.4 (3)
O3—C14—C15—O5	−179.1 (2)	C1—C2—N2—C6	−2.1 (3)
N3—C14—C15—O5	0.8 (3)	O2—C5—N2—C2	176.6 (2)
O3—C14—C15—O4	64.4 (3)	N1—C5—N2—C2	−4.4 (3)
N3—C14—C15—O4	−115.6 (2)	O2—C5—N2—C6	0.3 (3)
C21—C16—C17—C18	−0.6 (4)	N1—C5—N2—C6	179.4 (2)
O4—C16—C17—C18	−178.7 (2)	O3—C14—N3—C9	−0.9 (4)
C16—C17—C18—F5	176.2 (3)	C15—C14—N3—C9	179.1 (2)
C16—C17—C18—C19	−1.4 (4)	C8—C9—N3—C14	10.5 (4)
F5—C18—C19—C20	−175.1 (3)	C10—C9—N3—C14	−171.3 (2)
C17—C18—C19—C20	2.5 (4)	C21—C16—O4—C15	19.0 (3)
C18—C19—C20—F5'	160.7 (5)	C17—C16—O4—C15	−163.0 (2)
C18—C19—C20—C21	−1.6 (5)	O5—C15—O4—C16	142.56 (19)
O4—C16—C21—C20	179.2 (2)	C14—C15—O4—C16	−100.2 (2)
C17—C16—C21—C20	1.4 (4)	C27—C22—O5—C15	0.3 (4)
F5'—C20—C21—C16	−163.5 (5)	C23—C22—O5—C15	−179.3 (2)
C19—C20—C21—C16	−0.3 (5)	O4—C15—O5—C22	−76.2 (3)
C27—C22—C23—C24	−1.4 (4)	C14—C15—O5—C22	166.5 (2)
O5—C22—C23—C24	178.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O3	0.93	2.31	2.896 (3)	121
C6—H6C···F2	0.96	2.37	3.046 (4)	127
N3—H3A···O5	0.85 (4)	2.07 (4)	2.545 (2)	115 (3)

N3—H3A···Cl1	0.85 (4)	2.44 (4)	2.9074 (19)	115 (3)

Fig. 1