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3'-(4-Chlorobenzoyl)-4'-(4-chlorophenyl)-1'-methylspiro[indoline-3,2'-pyrrolidin]-2-one

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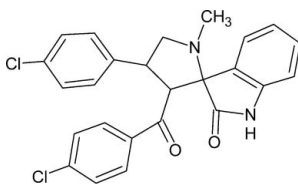
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.041; wR factor = 0.114; data-to-parameter ratio = 18.5.

In the title compound, $\text{C}_{25}\text{H}_{20}\text{Cl}_2\text{N}_2\text{O}_2$, the pyrrolidine ring adopts an envelope conformation and the best plane through the five ring atoms makes a dihedral angle of $87.03(8)^\circ$ with the indoline ring. Molecules are connected by pairs of $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into centrosymmetric dimers with an $R_2^2(8)$ graph-set ring motif. $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds stabilize the crystal structure.

Related literature

For substituted pyrrolidine compounds, see: Coldham & Hufton (2005). For graph-set notation of hydrogen bonds, see: Bernstein *et al.* (1995).



Experimental

Crystal data

 $\text{C}_{25}\text{H}_{20}\text{Cl}_2\text{N}_2\text{O}_2$ $M_r = 451.33$

Monoclinic, $P2_1/c$
 $a = 11.4139(2)$ Å
 $b = 11.6957(2)$ Å
 $c = 16.5262(2)$ Å
 $\beta = 102.037(1)^\circ$
 $V = 2157.64(6)$ Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.33$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART APEXII area-detector diffractometer
20528 measured reflections

5426 independent reflections
3812 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.114$
 $S = 1.03$
5426 reflections
293 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.44$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|----------|-------------|-------------|---------------|
| $\text{N2}-\text{H2A}\cdots\text{O2}^i$ | 0.85 (2) | 2.06 (2) | 2.876 (2) | 160 |
| $\text{C24}-\text{H24}\cdots\text{O1}^{ii}$ | 0.93 | 2.42 | 3.104 (2) | 130 |

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

TS and DV thank the TBI X-ray facility, CAS in Crystallography and Biophysics, University of Madras, India, for the data collection. TS also thanks the DST for an Inspire fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5687).

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supporting information

Acta Cryst. (2011). E67, o3128 [doi:10.1107/S1600536811044618]

3'-(4-Chlorobenzoyl)-4'-(4-chlorophenyl)-1'-methylspiro[indoline-3,2'-pyrrolidin]-2-one

T. Srinivasan, S. Suhitha, S. Purushothaman, R. Raghunathan and D. Velmurugan

S1. Comment

Substituted pyrrolidine compounds are an important class of heterocyclic compounds with wide spread applications to the synthesis of biologically active compounds and natural products (Coldham & Hufton, 2005).

The indoline ring is essentially planar with a maximum deviation of 0.0594 (16)Å for atom C12. The oxygen atom O2 deviates with the value of 0.0566 (13)Å from the indoline ring. The phenyl ring of chlorophenyl group makes a dihedral angle of 79.68 (9)° and 20.47 (7)° with the pyrrolidin ring and indoline ring system. The phenyl ring of chlorobenzaldehyde group makes a dihedral angle of 71.39 (9)° and 35.17 (8)° with the pyrrolidin ring and indoline ring system, respectively.

The pyrrolidin ring adopts an *envelope* conformation. The pyrrolidin ring makes a dihedral angle of 87.03 (8)° with the indoline ring system. The crystal structure is stabilized by C—H...O and N—H...O hydrogen bonds resulting in R²₂(16) and R²₂(8) graph-set ring motifs (Bernstein *et al.*, 1995).

S2. Experimental

A solution of (E)-1,3-bis(4-chlorophenyl)prop-2-en-1-one (2 mmol), isatin (1 eq.) and sarcosine (1 eq.) was refluxed in dry toluene for 8 hrs at 110°C using Dean-Stark apparatus. After the completion of reaction as indicated by TLC, toluene was evaporated under reduced pressure. The crude product was purified by column chromatography using hexane: EtOAc (8:2) as eluent.

S3. Refinement

The hydrogen atoms were placed in calculated positions with C—H = 0.93Å to 1.00Å and refined in the riding model with fixed isotropic displacement parameters: $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl group and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for other H atoms.

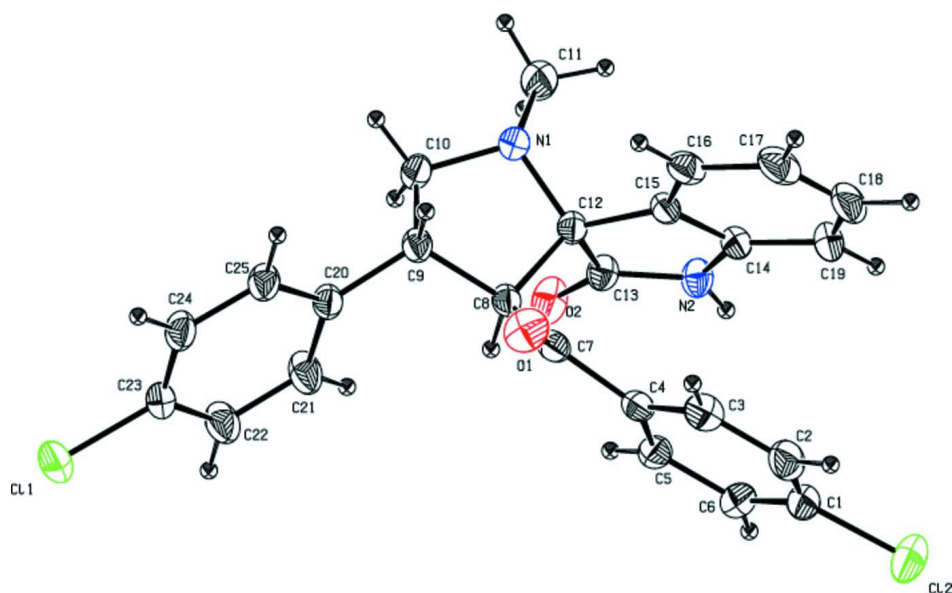


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

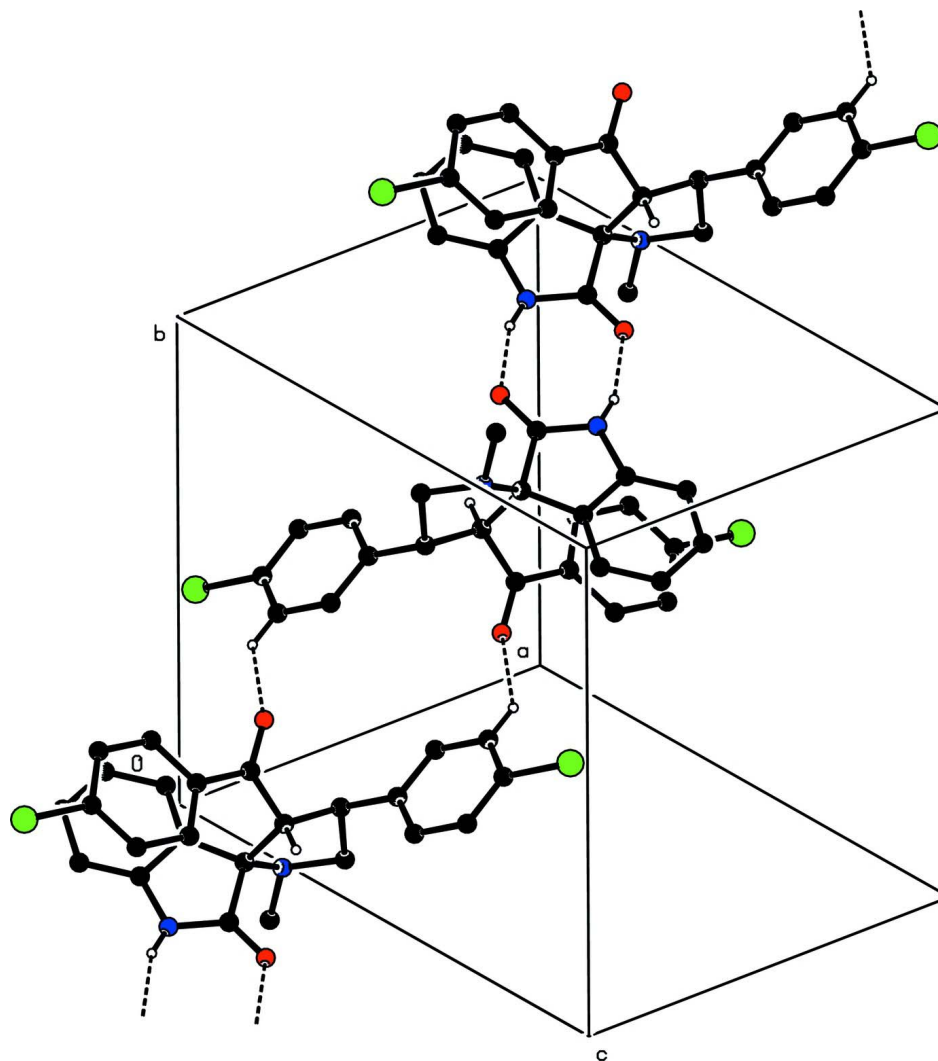


Figure 2

The crystal packing of the title compound viewed down *b* axis, showing the hydrogen bonds resulting in $R^2_2(16)$ and $R^2_2(8)$ graph-set ring motifs; H-atoms not involved in H-bonds have been excluded for clarity.

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Crystal data

$C_{25}H_{20}Cl_2N_2O_2$

$M_r = 451.33$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.4139(2) \text{ \AA}$

$b = 11.6957(2) \text{ \AA}$

$c = 16.5262(2) \text{ \AA}$

$\beta = 102.037(1)^\circ$

$V = 2157.64(6) \text{ \AA}^3$

$Z = 4$

$F(000) = 936$

$D_x = 1.389 \text{ Mg m}^{-3}$

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

Cell parameters from 5426 reflections

$\theta = 1.8\text{--}28.4^\circ$

$\mu = 0.33 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

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

Data collection

Bruker SMART APEXII area-detector
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 ω and φ scans
20528 measured reflections
5426 independent reflections

3812 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 28.4^\circ$, $\theta_{\text{min}} = 1.8^\circ$
 $h = -15 \rightarrow 13$
 $k = -15 \rightarrow 15$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.114$
 $S = 1.03$
5426 reflections
293 parameters
0 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.5071P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.44 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|--------------|----------------------------------|
| C11 | -0.14204 (5) | 0.56050 (5) | 0.16763 (3) | 0.06775 (17) |
| C12 | 0.85262 (5) | 0.60950 (6) | 0.62529 (4) | 0.0862 (2) |
| C9 | 0.11880 (14) | 0.73473 (15) | 0.50025 (9) | 0.0400 (4) |
| N2 | 0.48172 (13) | 0.92400 (12) | 0.60195 (9) | 0.0433 (3) |
| C15 | 0.37099 (14) | 0.80302 (13) | 0.66407 (8) | 0.0367 (3) |
| C7 | 0.31713 (14) | 0.62491 (14) | 0.54566 (9) | 0.0394 (3) |
| O2 | 0.34978 (11) | 0.96763 (11) | 0.48075 (8) | 0.0564 (3) |
| N1 | 0.17789 (11) | 0.88494 (12) | 0.59138 (8) | 0.0420 (3) |
| C8 | 0.25585 (13) | 0.73727 (14) | 0.51710 (9) | 0.0359 (3) |
| C12 | 0.29245 (13) | 0.83649 (13) | 0.58229 (8) | 0.0350 (3) |
| C20 | 0.05641 (13) | 0.69085 (15) | 0.41599 (9) | 0.0407 (4) |
| C23 | -0.06461 (15) | 0.61146 (16) | 0.26300 (10) | 0.0472 (4) |
| O1 | 0.25970 (12) | 0.54417 (11) | 0.56163 (9) | 0.0602 (3) |
| C4 | 0.45034 (14) | 0.61803 (13) | 0.55866 (9) | 0.0381 (3) |
| C13 | 0.37572 (14) | 0.91885 (14) | 0.54743 (9) | 0.0396 (3) |
| C14 | 0.48245 (14) | 0.85308 (14) | 0.67070 (9) | 0.0402 (3) |

| | | | | |
|------|---------------|--------------|--------------|------------|
| C10 | 0.08849 (14) | 0.85794 (16) | 0.51710 (10) | 0.0457 (4) |
| H10A | 0.0963 | 0.9076 | 0.4715 | 0.055* |
| H10B | 0.0079 | 0.8643 | 0.5270 | 0.055* |
| C5 | 0.51767 (14) | 0.68787 (15) | 0.51797 (9) | 0.0429 (4) |
| H5 | 0.4790 | 0.7376 | 0.4771 | 0.052* |
| C25 | -0.04115 (14) | 0.61909 (16) | 0.40920 (10) | 0.0459 (4) |
| H25 | -0.0664 | 0.5969 | 0.4568 | 0.055* |
| C1 | 0.69779 (16) | 0.61090 (17) | 0.59772 (11) | 0.0533 (4) |
| C24 | -0.10233 (15) | 0.57939 (16) | 0.33323 (10) | 0.0484 (4) |
| H24 | -0.1682 | 0.5315 | 0.3298 | 0.058* |
| C6 | 0.64165 (15) | 0.68453 (17) | 0.53744 (11) | 0.0506 (4) |
| H6 | 0.6862 | 0.7316 | 0.5100 | 0.061* |
| C22 | 0.03220 (16) | 0.68206 (19) | 0.26713 (10) | 0.0593 (5) |
| H22 | 0.0576 | 0.7029 | 0.2193 | 0.071* |
| C16 | 0.34817 (17) | 0.73153 (15) | 0.72517 (9) | 0.0465 (4) |
| H16 | 0.2726 | 0.6999 | 0.7218 | 0.056* |
| C2 | 0.63333 (18) | 0.53729 (17) | 0.63664 (11) | 0.0570 (5) |
| H2 | 0.6726 | 0.4854 | 0.6757 | 0.068* |
| C17 | 0.4410 (2) | 0.70793 (18) | 0.79193 (10) | 0.0600 (5) |
| H17 | 0.4278 | 0.6597 | 0.8339 | 0.072* |
| C3 | 0.50996 (17) | 0.54119 (15) | 0.61720 (10) | 0.0500 (4) |
| H3 | 0.4661 | 0.4918 | 0.6436 | 0.060* |
| C21 | 0.09178 (16) | 0.72204 (18) | 0.34360 (10) | 0.0563 (5) |
| H21 | 0.1569 | 0.7708 | 0.3465 | 0.068* |
| C19 | 0.57585 (17) | 0.82942 (18) | 0.73636 (10) | 0.0556 (5) |
| H19 | 0.6512 | 0.8619 | 0.7400 | 0.067* |
| C18 | 0.5529 (2) | 0.75563 (19) | 0.79644 (11) | 0.0658 (6) |
| H18 | 0.6143 | 0.7376 | 0.8411 | 0.079* |
| C11 | 0.18210 (18) | 1.00343 (17) | 0.61905 (12) | 0.0593 (5) |
| H11A | 0.1973 | 1.0524 | 0.5758 | 0.089* |
| H11B | 0.2450 | 1.0123 | 0.6672 | 0.089* |
| H11C | 0.1068 | 1.0236 | 0.6324 | 0.089* |
| H2A | 0.5428 (19) | 0.9548 (17) | 0.5892 (12) | 0.059 (6)* |
| H8 | 0.2804 (14) | 0.7597 (13) | 0.4670 (10) | 0.037 (4)* |
| H9 | 0.0928 (14) | 0.6848 (14) | 0.5430 (10) | 0.039 (4)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|-------------|------------|-------------|-------------|-------------|
| C11 | 0.0563 (3) | 0.0957 (4) | 0.0465 (2) | -0.0108 (3) | 0.0000 (2) | -0.0216 (2) |
| C12 | 0.0442 (3) | 0.1103 (5) | 0.0945 (4) | 0.0194 (3) | -0.0074 (3) | -0.0141 (4) |
| C9 | 0.0320 (8) | 0.0555 (10) | 0.0323 (7) | -0.0082 (7) | 0.0064 (6) | 0.0019 (7) |
| N2 | 0.0359 (7) | 0.0450 (8) | 0.0466 (7) | -0.0103 (6) | 0.0036 (6) | 0.0004 (6) |
| C15 | 0.0392 (8) | 0.0399 (8) | 0.0291 (6) | 0.0034 (7) | 0.0031 (6) | -0.0034 (6) |
| C7 | 0.0436 (9) | 0.0440 (9) | 0.0317 (7) | -0.0064 (7) | 0.0103 (6) | -0.0045 (6) |
| O2 | 0.0453 (7) | 0.0658 (8) | 0.0553 (7) | -0.0057 (6) | 0.0045 (6) | 0.0267 (6) |
| N1 | 0.0338 (7) | 0.0526 (8) | 0.0384 (7) | 0.0027 (6) | 0.0051 (5) | -0.0035 (6) |
| C8 | 0.0311 (7) | 0.0481 (9) | 0.0286 (6) | -0.0063 (6) | 0.0061 (6) | 0.0009 (6) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|-------------|-------------|
| C12 | 0.0321 (8) | 0.0400 (8) | 0.0323 (7) | -0.0030 (6) | 0.0052 (6) | 0.0020 (6) |
| C20 | 0.0323 (8) | 0.0534 (9) | 0.0351 (7) | -0.0051 (7) | 0.0042 (6) | 0.0016 (7) |
| C23 | 0.0367 (9) | 0.0630 (11) | 0.0385 (8) | -0.0009 (8) | -0.0002 (7) | -0.0070 (8) |
| O1 | 0.0583 (8) | 0.0485 (7) | 0.0773 (9) | -0.0123 (6) | 0.0220 (7) | 0.0039 (6) |
| C4 | 0.0425 (9) | 0.0401 (8) | 0.0315 (7) | 0.0011 (7) | 0.0072 (6) | -0.0053 (6) |
| C13 | 0.0355 (8) | 0.0408 (8) | 0.0416 (8) | -0.0027 (7) | 0.0057 (6) | 0.0040 (6) |
| C14 | 0.0388 (8) | 0.0441 (9) | 0.0353 (7) | 0.0022 (7) | 0.0022 (6) | -0.0070 (6) |
| C10 | 0.0312 (8) | 0.0642 (11) | 0.0405 (8) | 0.0012 (7) | 0.0049 (6) | 0.0004 (7) |
| C5 | 0.0403 (9) | 0.0534 (10) | 0.0358 (7) | 0.0054 (7) | 0.0095 (6) | 0.0036 (7) |
| C25 | 0.0345 (8) | 0.0643 (11) | 0.0385 (8) | -0.0076 (8) | 0.0069 (6) | 0.0054 (7) |
| C1 | 0.0427 (10) | 0.0620 (12) | 0.0509 (9) | 0.0114 (9) | 0.0000 (8) | -0.0145 (9) |
| C24 | 0.0331 (8) | 0.0616 (11) | 0.0479 (9) | -0.0104 (8) | 0.0022 (7) | -0.0002 (8) |
| C6 | 0.0394 (9) | 0.0638 (11) | 0.0500 (9) | 0.0034 (8) | 0.0121 (7) | -0.0015 (8) |
| C22 | 0.0511 (11) | 0.0909 (15) | 0.0356 (8) | -0.0186 (10) | 0.0085 (7) | 0.0009 (9) |
| C16 | 0.0585 (11) | 0.0490 (9) | 0.0337 (7) | 0.0051 (8) | 0.0131 (7) | 0.0009 (7) |
| C2 | 0.0621 (12) | 0.0564 (11) | 0.0459 (9) | 0.0184 (9) | -0.0036 (8) | -0.0010 (8) |
| C17 | 0.0856 (15) | 0.0617 (12) | 0.0319 (8) | 0.0163 (11) | 0.0102 (9) | 0.0049 (8) |
| C3 | 0.0617 (12) | 0.0435 (10) | 0.0450 (9) | 0.0041 (8) | 0.0115 (8) | 0.0025 (7) |
| C21 | 0.0464 (10) | 0.0823 (14) | 0.0395 (8) | -0.0263 (9) | 0.0070 (7) | 0.0000 (9) |
| C19 | 0.0455 (10) | 0.0719 (13) | 0.0424 (9) | 0.0046 (9) | -0.0070 (7) | -0.0127 (9) |
| C18 | 0.0732 (14) | 0.0810 (15) | 0.0340 (8) | 0.0263 (12) | -0.0098 (9) | -0.0059 (9) |
| C11 | 0.0514 (11) | 0.0609 (12) | 0.0614 (11) | 0.0097 (9) | 0.0019 (9) | -0.0120 (9) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|-----------|
| C11—C23 | 1.7433 (16) | C14—C19 | 1.381 (2) |
| C12—C1 | 1.7306 (19) | C10—H10A | 0.9700 |
| C9—C20 | 1.515 (2) | C10—H10B | 0.9700 |
| C9—C10 | 1.521 (2) | C5—C6 | 1.385 (2) |
| C9—C8 | 1.531 (2) | C5—H5 | 0.9300 |
| C9—H9 | 1.007 (16) | C25—C24 | 1.383 (2) |
| N2—C13 | 1.351 (2) | C25—H25 | 0.9300 |
| N2—C14 | 1.405 (2) | C1—C6 | 1.371 (3) |
| N2—H2A | 0.85 (2) | C1—C2 | 1.376 (3) |
| C15—C16 | 1.377 (2) | C24—H24 | 0.9300 |
| C15—C14 | 1.384 (2) | C6—H6 | 0.9300 |
| C15—C12 | 1.5093 (19) | C22—C21 | 1.386 (2) |
| C7—O1 | 1.2096 (19) | C22—H22 | 0.9300 |
| C7—C4 | 1.493 (2) | C16—C17 | 1.389 (3) |
| C7—C8 | 1.517 (2) | C16—H16 | 0.9300 |
| O2—C13 | 1.2213 (19) | C2—C3 | 1.378 (3) |
| N1—C11 | 1.457 (2) | C2—H2 | 0.9300 |
| N1—C10 | 1.458 (2) | C17—C18 | 1.381 (3) |
| N1—C12 | 1.4612 (19) | C17—H17 | 0.9300 |
| C8—C12 | 1.579 (2) | C3—H3 | 0.9300 |
| C8—H8 | 0.964 (15) | C21—H21 | 0.9300 |
| C12—C13 | 1.546 (2) | C19—C18 | 1.381 (3) |
| C20—C25 | 1.380 (2) | C19—H19 | 0.9300 |

| | | | |
|-------------|-------------|---------------|-------------|
| C20—C21 | 1.389 (2) | C18—H18 | 0.9300 |
| C23—C22 | 1.370 (2) | C11—H11A | 0.9600 |
| C23—C24 | 1.372 (2) | C11—H11B | 0.9600 |
| C4—C5 | 1.388 (2) | C11—H11C | 0.9600 |
| C4—C3 | 1.390 (2) | | |
| C20—C9—C10 | 114.07 (14) | N1—C10—H10B | 111.3 |
| C20—C9—C8 | 116.12 (12) | C9—C10—H10B | 111.3 |
| C10—C9—C8 | 102.19 (13) | H10A—C10—H10B | 109.2 |
| C20—C9—H9 | 107.3 (9) | C6—C5—C4 | 120.88 (15) |
| C10—C9—H9 | 108.0 (9) | C6—C5—H5 | 119.6 |
| C8—C9—H9 | 108.8 (9) | C4—C5—H5 | 119.6 |
| C13—N2—C14 | 111.50 (14) | C20—C25—C24 | 121.60 (15) |
| C13—N2—H2A | 121.4 (13) | C20—C25—H25 | 119.2 |
| C14—N2—H2A | 125.7 (14) | C24—C25—H25 | 119.2 |
| C16—C15—C14 | 120.67 (14) | C6—C1—C2 | 121.22 (17) |
| C16—C15—C12 | 130.26 (15) | C6—C1—C12 | 119.63 (16) |
| C14—C15—C12 | 109.01 (13) | C2—C1—C12 | 119.16 (15) |
| O1—C7—C4 | 120.57 (15) | C23—C24—C25 | 119.21 (15) |
| O1—C7—C8 | 120.56 (15) | C23—C24—H24 | 120.4 |
| C4—C7—C8 | 118.76 (13) | C25—C24—H24 | 120.4 |
| C11—N1—C10 | 116.21 (14) | C1—C6—C5 | 119.13 (17) |
| C11—N1—C12 | 115.43 (13) | C1—C6—H6 | 120.4 |
| C10—N1—C12 | 108.29 (12) | C5—C6—H6 | 120.4 |
| C7—C8—C9 | 115.29 (13) | C23—C22—C21 | 119.11 (16) |
| C7—C8—C12 | 112.65 (12) | C23—C22—H22 | 120.4 |
| C9—C8—C12 | 104.67 (12) | C21—C22—H22 | 120.4 |
| C7—C8—H8 | 107.7 (9) | C15—C16—C17 | 118.25 (18) |
| C9—C8—H8 | 108.6 (9) | C15—C16—H16 | 120.9 |
| C12—C8—H8 | 107.7 (9) | C17—C16—H16 | 120.9 |
| N1—C12—C15 | 112.69 (12) | C1—C2—C3 | 119.36 (17) |
| N1—C12—C13 | 115.44 (13) | C1—C2—H2 | 120.3 |
| C15—C12—C13 | 101.46 (12) | C3—C2—H2 | 120.3 |
| N1—C12—C8 | 103.88 (11) | C18—C17—C16 | 120.42 (18) |
| C15—C12—C8 | 116.32 (13) | C18—C17—H17 | 119.8 |
| C13—C12—C8 | 107.41 (11) | C16—C17—H17 | 119.8 |
| C25—C20—C21 | 117.66 (14) | C2—C3—C4 | 120.78 (17) |
| C25—C20—C9 | 119.82 (13) | C2—C3—H3 | 119.6 |
| C21—C20—C9 | 122.51 (14) | C4—C3—H3 | 119.6 |
| C22—C23—C24 | 120.99 (15) | C22—C21—C20 | 121.43 (16) |
| C22—C23—C11 | 120.19 (13) | C22—C21—H21 | 119.3 |
| C24—C23—C11 | 118.82 (13) | C20—C21—H21 | 119.3 |
| C5—C4—C3 | 118.53 (15) | C18—C19—C14 | 117.30 (18) |
| C5—C4—C7 | 123.30 (14) | C18—C19—H19 | 121.3 |
| C3—C4—C7 | 118.11 (15) | C14—C19—H19 | 121.3 |
| O2—C13—N2 | 126.58 (15) | C17—C18—C19 | 121.72 (17) |
| O2—C13—C12 | 125.09 (14) | C17—C18—H18 | 119.1 |
| N2—C13—C12 | 108.29 (13) | C19—C18—H18 | 119.1 |

| | | | |
|-----------------|--------------|-----------------|--------------|
| C19—C14—C15 | 121.57 (16) | N1—C11—H11A | 109.5 |
| C19—C14—N2 | 128.82 (16) | N1—C11—H11B | 109.5 |
| C15—C14—N2 | 109.59 (13) | H11A—C11—H11B | 109.5 |
| N1—C10—C9 | 102.32 (13) | N1—C11—H11C | 109.5 |
| N1—C10—H10A | 111.3 | H11A—C11—H11C | 109.5 |
| C9—C10—H10A | 111.3 | H11B—C11—H11C | 109.5 |
| O1—C7—C8—C9 | -7.3 (2) | C15—C12—C13—N2 | 1.53 (16) |
| C4—C7—C8—C9 | 176.42 (12) | C8—C12—C13—N2 | -121.00 (14) |
| O1—C7—C8—C12 | 112.75 (16) | C16—C15—C14—C19 | 3.0 (2) |
| C4—C7—C8—C12 | -63.54 (16) | C12—C15—C14—C19 | -174.50 (15) |
| C20—C9—C8—C7 | -83.09 (17) | C16—C15—C14—N2 | -178.46 (14) |
| C10—C9—C8—C7 | 152.12 (12) | C12—C15—C14—N2 | 4.06 (17) |
| C20—C9—C8—C12 | 152.59 (13) | C13—N2—C14—C19 | 175.32 (17) |
| C10—C9—C8—C12 | 27.79 (14) | C13—N2—C14—C15 | -3.10 (19) |
| C11—N1—C12—C15 | 77.91 (17) | C11—N1—C10—C9 | 173.24 (14) |
| C10—N1—C12—C15 | -149.85 (13) | C12—N1—C10—C9 | 41.42 (15) |
| C11—N1—C12—C13 | -38.02 (18) | C20—C9—C10—N1 | -167.97 (12) |
| C10—N1—C12—C13 | 94.22 (15) | C8—C9—C10—N1 | -41.82 (14) |
| C11—N1—C12—C8 | -155.33 (13) | C3—C4—C5—C6 | -2.5 (2) |
| C10—N1—C12—C8 | -23.09 (15) | C7—C4—C5—C6 | 174.50 (15) |
| C16—C15—C12—N1 | 55.4 (2) | C21—C20—C25—C24 | -0.2 (3) |
| C14—C15—C12—N1 | -127.39 (14) | C9—C20—C25—C24 | 178.42 (16) |
| C16—C15—C12—C13 | 179.49 (16) | C22—C23—C24—C25 | -0.1 (3) |
| C14—C15—C12—C13 | -3.36 (16) | C11—C23—C24—C25 | 179.77 (14) |
| C16—C15—C12—C8 | -64.4 (2) | C20—C25—C24—C23 | 0.5 (3) |
| C14—C15—C12—C8 | 112.81 (14) | C2—C1—C6—C5 | 2.7 (3) |
| C7—C8—C12—N1 | -130.00 (12) | C12—C1—C6—C5 | -177.68 (13) |
| C9—C8—C12—N1 | -4.01 (14) | C4—C5—C6—C1 | 0.1 (3) |
| C7—C8—C12—C15 | -5.56 (17) | C24—C23—C22—C21 | -0.5 (3) |
| C9—C8—C12—C15 | 120.43 (14) | C11—C23—C22—C21 | 179.58 (17) |
| C7—C8—C12—C13 | 107.23 (14) | C14—C15—C16—C17 | -2.3 (2) |
| C9—C8—C12—C13 | -126.78 (12) | C12—C15—C16—C17 | 174.61 (16) |
| C10—C9—C20—C25 | -102.97 (18) | C6—C1—C2—C3 | -2.9 (3) |
| C8—C9—C20—C25 | 138.57 (16) | C12—C1—C2—C3 | 177.48 (14) |
| C10—C9—C20—C21 | 75.5 (2) | C15—C16—C17—C18 | 0.2 (3) |
| C8—C9—C20—C21 | -42.9 (2) | C1—C2—C3—C4 | 0.3 (3) |
| O1—C7—C4—C5 | 157.76 (16) | C5—C4—C3—C2 | 2.3 (2) |
| C8—C7—C4—C5 | -25.9 (2) | C7—C4—C3—C2 | -174.86 (15) |
| O1—C7—C4—C3 | -25.2 (2) | C23—C22—C21—C20 | 0.9 (3) |
| C8—C7—C4—C3 | 151.11 (14) | C25—C20—C21—C22 | -0.5 (3) |
| C14—N2—C13—O2 | -177.25 (17) | C9—C20—C21—C22 | -179.06 (19) |
| C14—N2—C13—C12 | 0.80 (18) | C15—C14—C19—C18 | -1.5 (3) |
| N1—C12—C13—O2 | -58.2 (2) | N2—C14—C19—C18 | -179.75 (17) |
| C15—C12—C13—O2 | 179.62 (16) | C16—C17—C18—C19 | 1.3 (3) |
| C8—C12—C13—O2 | 57.1 (2) | C14—C19—C18—C17 | -0.6 (3) |
| N1—C12—C13—N2 | 123.69 (14) | | |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N2—H2A \cdots O2 ⁱ | 0.85 (2) | 2.06 (2) | 2.876 (2) | 160 |
| C24—H24 \cdots O1 ⁱⁱ | 0.93 | 2.42 | 3.104 (2) | 130 |

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