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# *N*-(2-Chlorophenyl)-1-phenylformamido 3-(2-nitrophenyl)propanoate

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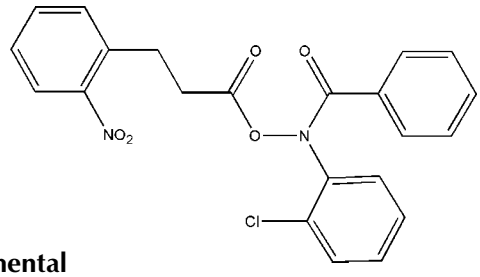
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.047; $wR$ factor = 0.114; data-to-parameter ratio = 13.6.

In the title molecule, $C_{22}H_{17}ClN_2O_5$, the nitro-substituted benzene ring makes a dihedral angle of 79.22 (1)° with the benzoyl ring and 53.03 (1)° with the chloro-substituted benzene ring. An intramolecular C—H···O hydrogen bond occurs. The crystal structure features weak C—H···Cl and C—H···O interactions.

## Related literature

For applications of hydroxamic acid derivatives, see: Noh *et al.* (2009); Zeng *et al.* (2003). For the preparation, see: Ayyangark *et al.* (1986).




## Experimental

### *Crystal data*

$C_{22}H_{17}ClN_2O_5$
$M_r$ = 424.83
Monoclinic, $P2_1/n$
$a$ = 14.698 (9) Å
$b$ = 8.030 (5) Å
$c$ = 17.495 (11) Å
$\beta$ = 103.059 (7)°
$V$ = 2011 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 296 K
0.26 × 0.23 × 0.22 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.943, $T_{max}$ = 0.952
8356 measured reflections
3697 independent reflections
2285 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
$S$ = 1.02
3697 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.26 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8$B$···Cl1$^{i}$ | 0.97 | 2.68 | 3.627 (3) | 167 |
| C7—H7$A$···O1$^{ii}$ | 0.97 | 2.60 | 3.520 (3) | 158 |
| C8—H8$A$···O2 | 0.97 | 2.47 | 3.092 (3) | 121 |
| C18—H18···O1$^{iii}$ | 0.93 | 2.62 | 3.517 (4) | 161 |
| C4—H4···O1$^{iv}$ | 0.93 | 2.64 | 3.468 (4) | 149 |

Symmetry codes: (i) $-x+2, -y+2, -z$; (ii) $-x+1, -y+1, -z$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $x, y+1, z$.

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2179).

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# supporting information

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## *N*-(2-Chlorophenyl)-1-phenylformamido 3-(2-nitrophenyl)propanoate

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### S1. Comment

Hydroxamic acid derivatives have received considerable attention in recent years as the result of the discovery of their role in the biochemical toxicology of many drugs and other chemicals. Thus, these compounds continue to attract much attention as potential biological agents (Noh *et al.*, 2009; Zeng *et al.*, 2003).

The title compound, $C_{22}H_{17}N_2O_5Cl$, was prepared according to the method described by Ayyangark *et al.* (1986). The molecule contains three branched chains with its centre placed at midpoint of the N2 atom (Fig. 1). The phenyl ring C1—C6 makes dihedral angles of 79.22 (1)° with the phenyl ring C17—C22, and 53.03 (1)° with the phenyl ring C10—C15.

The crystal structure features weak C—H···Cl and C—H···O interactions (Table 1).

### S2. Experimental

The title compound was prepared according to the method described by Ayyangark *et al.* (1986). The colourless crystals were grown from a solution of dichloromethane-methanol (1:3 *v*/*v*) by slow evaporation at room temperature.

### S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}$ = 1.2$U_{eq}$(C) for aromatic H atoms, and with C—H = 0.97 Å and $U_{iso}$ = 1.2$U_{eq}$(C) for methylene H atoms.

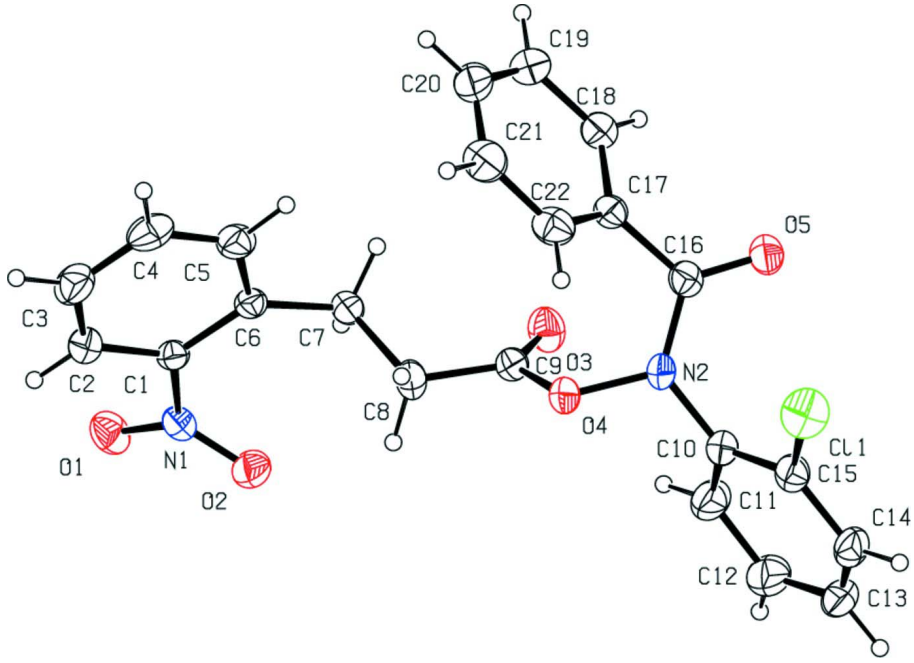


**Figure 1**

The molecular structure of the title compound with the atomic numbering and 30% probability displacement ellipsoids (H atoms are shown as small spheres of arbitrary radius).

## *N*-(2-Chlorophenyl)-1-phenylformamido 3-(2-nitrophenyl)propanoate

*Crystal data*

$C_{22}H_{17}ClN_2O_5$
$M_r = 424.83$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 14.698\ (9)$ Å
$b = 8.030\ (5)$ Å
$c = 17.495\ (11)$ Å
$\beta = 103.059\ (7)°$
$V = 2011\ (2)$ Å$^3$
$Z = 4$
$F(000) = 880$
$D_x = 1.403$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1690 reflections
$\theta = 2.4–22.2°$
$\mu = 0.23$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.26 × 0.23 × 0.22 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.943$, $T_{max} = 0.952$
8356 measured reflections
3697 independent reflections
2285 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.4°$
$h = -17\rightarrow13$
$k = -9\rightarrow9$
$l = -21\rightarrow19$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.114$
$S = 1.02$
3697 reflections

271 parameters
0 restraints
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.26$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.54356 (14) | 0.7597 (3) | −0.08505 (13) | 0.0364 (5) |
| C2 | 0.47799 (16) | 0.8218 (3) | −0.14815 (14) | 0.0499 (7) |
| H2 | 0.4370 | 0.7502 | −0.1809 | 0.060* |
| C3 | 0.47420 (19) | 0.9893 (4) | −0.16184 (17) | 0.0625 (8) |
| H3 | 0.4314 | 1.0326 | −0.2047 | 0.075* |
| C4 | 0.53416 (19) | 1.0939 (4) | −0.11187 (18) | 0.0626 (8) |
| H4 | 0.5323 | 1.2081 | −0.1210 | 0.075* |
| C5 | 0.59688 (16) | 1.0288 (3) | −0.04832 (16) | 0.0525 (7) |
| H5 | 0.6359 | 1.1014 | −0.0145 | 0.063* |
| C6 | 0.60438 (14) | 0.8602 (3) | −0.03261 (13) | 0.0375 (6) |
| C7 | 0.67502 (14) | 0.8013 (3) | 0.03913 (13) | 0.0441 (6) |
| H7A | 0.6520 | 0.7007 | 0.0590 | 0.053* |
| H7B | 0.6820 | 0.8856 | 0.0797 | 0.053* |
| C8 | 0.77017 (14) | 0.7660 (3) | 0.02151 (13) | 0.0457 (6) |
| H8A | 0.7677 | 0.6601 | −0.0056 | 0.055* |
| H8B | 0.7841 | 0.8517 | −0.0132 | 0.055* |
| C9 | 0.84611 (15) | 0.7607 (3) | 0.09349 (15) | 0.0417 (6) |
| C10 | 1.07421 (15) | 0.7137 (3) | 0.15039 (14) | 0.0456 (6) |
| C11 | 1.05317 (18) | 0.5495 (4) | 0.15897 (17) | 0.0646 (8) |
| H11 | 0.9922 | 0.5189 | 0.1592 | 0.077* |
| C12 | 1.1218 (2) | 0.4293 (4) | 0.16719 (17) | 0.0701 (9) |
| H12 | 1.1067 | 0.3178 | 0.1718 | 0.084* |
| C13 | 1.21242 (19) | 0.4745 (4) | 0.16857 (16) | 0.0627 (8) |
| H13 | 1.2590 | 0.3938 | 0.1756 | 0.075* |
| C14 | 1.23411 (17) | 0.6372 (4) | 0.15972 (14) | 0.0567 (7) |
| H14 | 1.2954 | 0.6674 | 0.1606 | 0.068* |
| C15 | 1.16538 (16) | 0.7572 (3) | 0.14945 (13) | 0.0467 (6) |
| C16 | 0.99784 (16) | 0.9673 (3) | 0.18933 (15) | 0.0428 (6) |
| C17 | 0.92056 (15) | 1.0900 (3) | 0.16295 (14) | 0.0414 (6) |
| C18 | 0.86650 (17) | 1.1325 (3) | 0.21517 (15) | 0.0527 (7) |
| H18 | 0.8794 | 1.0861 | 0.2652 | 0.063* |

| | | | | |
|---|---|---|---|---|
| C19 | 0.79360 (18) | 1.2432 (4) | 0.19365 (18) | 0.0616 (8) |
| H19 | 0.7567 | 1.2696 | 0.2287 | 0.074* |
| C20 | 0.7755 (2) | 1.3147 (4) | 0.12042 (19) | 0.0677 (8) |
| H20 | 0.7261 | 1.3891 | 0.1059 | 0.081* |
| C21 | 0.8295 (2) | 1.2771 (4) | 0.06901 (18) | 0.0666 (8) |
| H21 | 0.8176 | 1.3274 | 0.0199 | 0.080* |
| C22 | 0.90226 (18) | 1.1643 (3) | 0.08966 (16) | 0.0558 (7) |
| H22 | 0.9388 | 1.1385 | 0.0543 | 0.067* |
| Cl1 | 1.19330 (5) | 0.96079 (10) | 0.13393 (4) | 0.0716 (3) |
| N1 | 0.54447 (14) | 0.5788 (3) | −0.07543 (11) | 0.0415 (5) |
| N2 | 1.00361 (12) | 0.8386 (3) | 0.13960 (12) | 0.0529 (6) |
| O1 | 0.46940 (12) | 0.5048 (2) | −0.09402 (10) | 0.0596 (5) |
| O2 | 0.61882 (12) | 0.5081 (2) | −0.05065 (10) | 0.0556 (5) |
| O3 | 0.84162 (11) | 0.7242 (2) | 0.15847 (10) | 0.0573 (5) |
| O4 | 0.92840 (9) | 0.8124 (2) | 0.07409 (9) | 0.0457 (4) |
| O5 | 1.05461 (11) | 0.9793 (2) | 0.25171 (10) | 0.0536 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0354 (12) | 0.0330 (15) | 0.0410 (14) | 0.0018 (10) | 0.0094 (10) | −0.0036 (11) |
| C2 | 0.0460 (14) | 0.0504 (19) | 0.0493 (16) | 0.0066 (12) | 0.0021 (12) | −0.0035 (13) |
| C3 | 0.0597 (17) | 0.063 (2) | 0.0625 (19) | 0.0194 (15) | 0.0083 (14) | 0.0084 (16) |
| C4 | 0.0661 (18) | 0.0404 (17) | 0.085 (2) | 0.0127 (14) | 0.0254 (17) | 0.0051 (17) |
| C5 | 0.0465 (15) | 0.0398 (17) | 0.071 (2) | −0.0037 (12) | 0.0134 (14) | −0.0118 (14) |
| C6 | 0.0331 (12) | 0.0378 (16) | 0.0429 (14) | −0.0005 (10) | 0.0113 (11) | −0.0061 (12) |
| C7 | 0.0376 (13) | 0.0526 (17) | 0.0412 (14) | −0.0013 (11) | 0.0068 (11) | −0.0110 (12) |
| C8 | 0.0360 (12) | 0.0627 (18) | 0.0366 (14) | −0.0044 (12) | 0.0041 (10) | 0.0003 (13) |
| C9 | 0.0373 (13) | 0.0398 (16) | 0.0467 (16) | −0.0008 (11) | 0.0066 (11) | −0.0053 (13) |
| C10 | 0.0365 (13) | 0.0526 (18) | 0.0450 (15) | 0.0034 (12) | 0.0037 (11) | −0.0065 (13) |
| C11 | 0.0442 (15) | 0.057 (2) | 0.090 (2) | 0.0011 (14) | 0.0109 (15) | −0.0104 (17) |
| C12 | 0.068 (2) | 0.052 (2) | 0.087 (2) | 0.0074 (16) | 0.0099 (17) | −0.0058 (17) |
| C13 | 0.0543 (18) | 0.074 (2) | 0.0562 (18) | 0.0248 (16) | 0.0042 (13) | −0.0037 (16) |
| C14 | 0.0394 (14) | 0.087 (2) | 0.0448 (16) | 0.0105 (15) | 0.0123 (12) | −0.0005 (16) |
| C15 | 0.0445 (14) | 0.0617 (19) | 0.0346 (14) | 0.0025 (13) | 0.0103 (11) | 0.0032 (13) |
| C16 | 0.0369 (13) | 0.0468 (16) | 0.0459 (15) | −0.0082 (11) | 0.0119 (12) | −0.0032 (13) |
| C17 | 0.0410 (13) | 0.0376 (15) | 0.0448 (15) | −0.0030 (11) | 0.0081 (11) | −0.0044 (12) |
| C18 | 0.0545 (15) | 0.0526 (18) | 0.0480 (16) | 0.0045 (13) | 0.0056 (13) | −0.0054 (14) |
| C19 | 0.0560 (16) | 0.063 (2) | 0.066 (2) | 0.0100 (14) | 0.0133 (15) | −0.0114 (17) |
| C20 | 0.0652 (18) | 0.050 (2) | 0.078 (2) | 0.0126 (14) | −0.0057 (17) | −0.0105 (17) |
| C21 | 0.088 (2) | 0.0488 (19) | 0.0571 (19) | 0.0096 (16) | 0.0036 (17) | 0.0065 (15) |
| C22 | 0.0701 (18) | 0.0462 (18) | 0.0515 (17) | −0.0007 (14) | 0.0145 (14) | 0.0006 (14) |
| Cl1 | 0.0704 (5) | 0.0792 (6) | 0.0717 (5) | −0.0083 (4) | 0.0297 (4) | 0.0167 (4) |
| N1 | 0.0432 (12) | 0.0438 (14) | 0.0372 (11) | −0.0062 (11) | 0.0083 (9) | −0.0052 (10) |
| N2 | 0.0325 (11) | 0.0582 (15) | 0.0599 (14) | 0.0049 (10) | −0.0067 (10) | −0.0175 (12) |
| O1 | 0.0559 (11) | 0.0587 (13) | 0.0631 (12) | −0.0200 (9) | 0.0111 (9) | −0.0105 (10) |
| O2 | 0.0537 (11) | 0.0443 (12) | 0.0655 (12) | 0.0071 (8) | 0.0063 (9) | −0.0012 (9) |
| O3 | 0.0567 (10) | 0.0718 (14) | 0.0408 (11) | −0.0034 (9) | 0.0059 (8) | 0.0072 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4 | 0.0332 (8) | 0.0530 (11) | 0.0480 (10) | −0.0028 (7) | 0.0028 (8) | −0.0075 (8) |
| O5 | 0.0436 (9) | 0.0657 (13) | 0.0483 (11) | −0.0010 (8) | 0.0040 (8) | −0.0058 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.384 (3) | C12—C13 | 1.376 (4) |
| C1—C6 | 1.386 (3) | C12—H12 | 0.9300 |
| C1—N1 | 1.462 (3) | C13—C14 | 1.362 (4) |
| C2—C3 | 1.365 (3) | C13—H13 | 0.9300 |
| C2—H2 | 0.9300 | C14—C15 | 1.378 (3) |
| C3—C4 | 1.378 (4) | C14—H14 | 0.9300 |
| C3—H3 | 0.9300 | C15—Cl1 | 1.722 (3) |
| C4—C5 | 1.377 (4) | C16—O5 | 1.219 (3) |
| C4—H4 | 0.9300 | C16—N2 | 1.365 (3) |
| C5—C6 | 1.381 (3) | C16—C17 | 1.496 (3) |
| C5—H5 | 0.9300 | C17—C18 | 1.382 (3) |
| C6—C7 | 1.513 (3) | C17—C22 | 1.384 (3) |
| C7—C8 | 1.525 (3) | C18—C19 | 1.377 (4) |
| C7—H7A | 0.9700 | C18—H18 | 0.9300 |
| C7—H7B | 0.9700 | C19—C20 | 1.374 (4) |
| C8—C9 | 1.483 (3) | C19—H19 | 0.9300 |
| C8—H8A | 0.9700 | C20—C21 | 1.362 (4) |
| C8—H8B | 0.9700 | C20—H20 | 0.9300 |
| C9—O3 | 1.190 (3) | C21—C22 | 1.386 (4) |
| C9—O4 | 1.391 (3) | C21—H21 | 0.9300 |
| C10—C11 | 1.370 (4) | C22—H22 | 0.9300 |
| C10—C15 | 1.388 (3) | N1—O2 | 1.221 (2) |
| C10—N2 | 1.425 (3) | N1—O1 | 1.230 (2) |
| C11—C12 | 1.380 (4) | N2—O4 | 1.417 (2) |
| C11—H11 | 0.9300 | | |

| | | | |
|---|---|---|---|
| C2—C1—C6 | 123.2 (2) | C13—C12—H12 | 120.0 |
| C2—C1—N1 | 115.9 (2) | C11—C12—H12 | 120.0 |
| C6—C1—N1 | 121.0 (2) | C14—C13—C12 | 120.1 (3) |
| C3—C2—C1 | 119.2 (2) | C14—C13—H13 | 119.9 |
| C3—C2—H2 | 120.4 | C12—C13—H13 | 119.9 |
| C1—C2—H2 | 120.4 | C13—C14—C15 | 120.1 (3) |
| C2—C3—C4 | 119.6 (3) | C13—C14—H14 | 119.9 |
| C2—C3—H3 | 120.2 | C15—C14—H14 | 119.9 |
| C4—C3—H3 | 120.2 | C14—C15—C10 | 120.3 (3) |
| C5—C4—C3 | 119.8 (3) | C14—C15—Cl1 | 119.4 (2) |
| C5—C4—H4 | 120.1 | C10—C15—Cl1 | 120.4 (2) |
| C3—C4—H4 | 120.1 | O5—C16—N2 | 120.1 (2) |
| C4—C5—C6 | 122.8 (2) | O5—C16—C17 | 122.9 (2) |
| C4—C5—H5 | 118.6 | N2—C16—C17 | 117.0 (2) |
| C6—C5—H5 | 118.6 | C18—C17—C22 | 119.0 (2) |
| C5—C6—C1 | 115.4 (2) | C18—C17—C16 | 118.0 (2) |
| C5—C6—C7 | 118.7 (2) | C22—C17—C16 | 123.0 (2) |

| | | | |
|---|---|---|---|
| C1—C6—C7 | 125.9 (2) | C19—C18—C17 | 120.4 (3) |
| C6—C7—C8 | 112.28 (19) | C19—C18—H18 | 119.8 |
| C6—C7—H7A | 109.1 | C17—C18—H18 | 119.8 |
| C8—C7—H7A | 109.1 | C20—C19—C18 | 120.0 (3) |
| C6—C7—H7B | 109.1 | C20—C19—H19 | 120.0 |
| C8—C7—H7B | 109.1 | C18—C19—H19 | 120.0 |
| H7A—C7—H7B | 107.9 | C21—C20—C19 | 120.3 (3) |
| C9—C8—C7 | 112.48 (19) | C21—C20—H20 | 119.9 |
| C9—C8—H8A | 109.1 | C19—C20—H20 | 119.9 |
| C7—C8—H8A | 109.1 | C20—C21—C22 | 120.3 (3) |
| C9—C8—H8B | 109.1 | C20—C21—H21 | 119.9 |
| C7—C8—H8B | 109.1 | C22—C21—H21 | 119.9 |
| H8A—C8—H8B | 107.8 | C17—C22—C21 | 120.0 (3) |
| O3—C9—O4 | 123.0 (2) | C17—C22—H22 | 120.0 |
| O3—C9—C8 | 128.7 (2) | C21—C22—H22 | 120.0 |
| O4—C9—C8 | 108.3 (2) | O2—N1—O1 | 123.2 (2) |
| C11—C10—C15 | 119.0 (2) | O2—N1—C1 | 119.14 (19) |
| C11—C10—N2 | 121.1 (2) | O1—N1—C1 | 117.7 (2) |
| C15—C10—N2 | 119.8 (2) | C16—N2—O4 | 118.59 (18) |
| C10—C11—C12 | 120.5 (3) | C16—N2—C10 | 126.6 (2) |
| C10—C11—H11 | 119.8 | O4—N2—C10 | 114.47 (18) |
| C12—C11—H11 | 119.8 | C9—O4—N2 | 114.17 (17) |
| C13—C12—C11 | 120.0 (3) | | |

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| C6—C1—C2—C3 | 2.3 (4) | N2—C16—C17—C18 | 131.7 (2) |
| N1—C1—C2—C3 | −178.7 (2) | O5—C16—C17—C22 | 129.7 (3) |
| C1—C2—C3—C4 | −1.4 (4) | N2—C16—C17—C22 | −49.6 (3) |
| C2—C3—C4—C5 | −0.4 (4) | C22—C17—C18—C19 | 2.1 (4) |
| C3—C4—C5—C6 | 1.4 (4) | C16—C17—C18—C19 | −179.1 (2) |
| C4—C5—C6—C1 | −0.5 (3) | C17—C18—C19—C20 | −1.3 (4) |
| C4—C5—C6—C7 | −179.5 (2) | C18—C19—C20—C21 | −0.2 (4) |
| C2—C1—C6—C5 | −1.4 (3) | C19—C20—C21—C22 | 1.1 (4) |
| N1—C1—C6—C5 | 179.72 (19) | C18—C17—C22—C21 | −1.2 (4) |
| C2—C1—C6—C7 | 177.5 (2) | C16—C17—C22—C21 | −179.9 (2) |
| N1—C1—C6—C7 | −1.4 (3) | C20—C21—C22—C17 | −0.4 (4) |
| C5—C6—C7—C8 | −89.7 (3) | C2—C1—N1—O2 | 145.1 (2) |
| C1—C6—C7—C8 | 91.5 (3) | C6—C1—N1—O2 | −35.9 (3) |
| C6—C7—C8—C9 | 161.9 (2) | C2—C1—N1—O1 | −33.9 (3) |
| C7—C8—C9—O3 | 27.9 (4) | C6—C1—N1—O1 | 145.1 (2) |
| C7—C8—C9—O4 | −150.2 (2) | O5—C16—N2—O4 | 169.69 (19) |
| C15—C10—C11—C12 | 0.5 (4) | C17—C16—N2—O4 | −11.0 (3) |
| N2—C10—C11—C12 | 178.2 (2) | O5—C16—N2—C10 | −3.3 (4) |
| C10—C11—C12—C13 | 1.5 (4) | C17—C16—N2—C10 | 176.0 (2) |
| C11—C12—C13—C14 | −1.8 (4) | C11—C10—N2—C16 | 116.1 (3) |
| C12—C13—C14—C15 | 0.1 (4) | C15—C10—N2—C16 | −66.3 (3) |
| C13—C14—C15—C10 | 1.9 (4) | C11—C10—N2—O4 | −57.2 (3) |
| C13—C14—C15—Cl1 | −177.1 (2) | C15—C10—N2—O4 | 120.5 (2) |
| C11—C10—C15—C14 | −2.2 (4) | O3—C9—O4—N2 | −7.8 (3) |

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| N2—C10—C15—C14 | −179.9 (2) | C8—C9—O4—N2 | 170.50 (18) |
| C11—C10—C15—Cl1 | 176.8 (2) | C16—N2—O4—C9 | −67.4 (3) |
| N2—C10—C15—Cl1 | −0.9 (3) | C10—N2—O4—C9 | 106.5 (2) |
| O5—C16—C17—C18 | −49.0 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8*B*···Cl1$^{i}$ | 0.97 | 2.68 | 3.627 (3) | 167 |
| C7—H7*A*···O1$^{ii}$ | 0.97 | 2.60 | 3.520 (3) | 158 |
| C8—H8*A*···O2 | 0.97 | 2.47 | 3.092 (3) | 121 |
| C18—H18···O1$^{iii}$ | 0.93 | 2.62 | 3.517 (4) | 161 |
| C4—H4···O1$^{iv}$ | 0.93 | 2.64 | 3.468 (4) | 149 |

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*+1/2, −*y*+3/2, *z*+1/2; (iv) *x*, *y*+1, *z*.