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# *N*-(4-Chlorophenyl)-*N*′-{4-[(*Z*)-hydroxy(1-oxo-1,3-dihydro-2*H*-inden-2-ylidene)methyl]phenyl}urea

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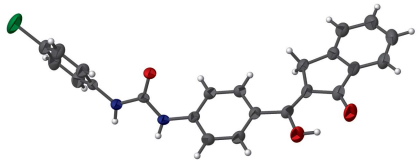
**Keywords:** crystal structure; 2,3-dihydro-1*H*-indene ring system; N—H···O hydrogen bonds; $\pi$–$\pi$ stacking interaction.

**CCDC reference**: 1846924

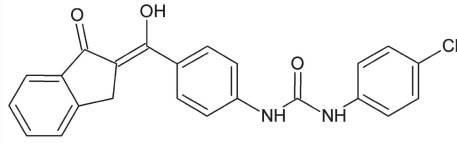
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{23}H_{17}ClN_2O_3$, the 2,3-dihydro-1*H*-indene ring system (r.m.s deviation = 0.004 Å) subtends dihedral angles of 81.12 (16) and 7.56 (14)° with the chlorophenyl and benzene rings, respectively. The molecular conformation features an intramolecular O—H···O hydrogen bond, forming an $S(6)$ ring motif. In the crystal, molecules are linked by N—H···O hydrogen bonds generating [100] chains featuring $R_1^2(6)$ loops. Weak aromatic $\pi$–$\pi$ stacking [centroid–centroid distance = 3.656 (2) Å] is also oberved.

**3D view**



**Chemical scheme**




## Structure description

Organic compounds containing the phenylurea unit are known to be valuable in terms of biological activity (Jiang *et al.*, 2016; Sikka *et al.*, 2015). As part of our studies in this area, we new report the crystal structure (Fig. 1) of the title compound (Gezegen *et al.*, 2017).

The 2,3-dihydro-1*H*-indene ring system (C15–C23) is essentially planar (r.m.s deviation = 0.004 Å), and is inclined at dihedral angles of 81.12 (16) and 7.56 (14)° with the chlorophenyl (C1–C6) and benzene (C8–C13) rings, respectively. The N—(C=O)—N plane involving the urea group is oriented at dihedral angles of 54.36 (17), 40.01 (15) and 56.15 (14)°, respectively, with the chlorophenyl ring, the benzene ring and the 2,3-dihydro-1*H*-indene ring system, respectively. The bond lengths and the bond angles of the title structure are within their normal ranges and are comparable to related structures (*e.g.* Yassine *et al.*, 2015; Mague *et al.*, 2015). The molecular conformation of the title

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2*O*···O3 | 0.89 (5) | 1.71 (5) | 2.543 (4) | 154 (5) |
| N1—H1*N*···O1$^{i}$ | 0.87 (6) | 2.03 (5) | 2.853 (4) | 158 (4) |
| N2—H2*N*···O1$^{i}$ | 0.81 (5) | 2.18 (5) | 2.904 (4) | 148 (4) |

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

compound is consolidated by an intramolecular O—H···O hydrogen bond, forming an $S(6)$ ring motif (Table 1).

In the crystal, adjacent molecules are linked by N—H···O hydrogen bonds (Fig. 2), generating infinite [100] chains incorporating $R_1^2(6)$ loops. In addition, weak aromatic $\pi$–$\pi$ stacking interactions are observed [$Cg1\cdots Cg4^{i}$ = 3.656 (2) Å; $Cg1$ and $Cg4$ are the centroids of the five- and six-membered rings (C15–C17/C22/C23 and C17–C22) of the 2,3-dihydro-1*H*-indene ring system, respectively; symmetry code: (i), $x+1$, $y$, $z$].

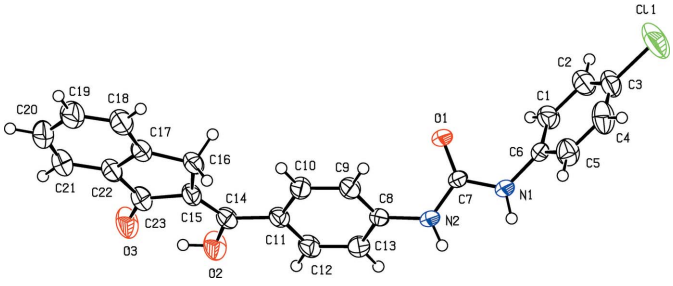



**Figure 1**
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

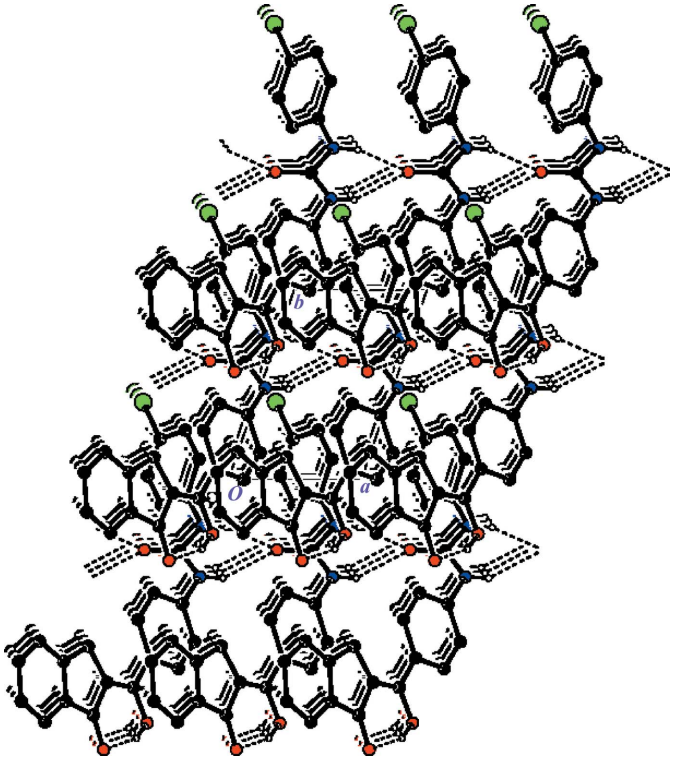



**Figure 2**
A view along the *c* axis of the crystal packing of the title compound. H bonds are shown as dashed lines and H atoms not involved in these interactions have been omitted for clarity.

## Synthesis and crystallization

For the sysnthesis of the title compound, see: Gezegen *et al.*, 2017. The crystals were grown from a DMSO solution by slow evaporation.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

The authors are indebted to the X-ray laboratory of Sinop University Scientific and Technological Applied and Research Center, Sinop, Turkey, for use of the X-ray diffractometer.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{23}H_{17}ClN_2O_3$ |
| $M_r$ | 404.84 |
| Crystal system, space group | Triclinic, *P*1 |
| Temperature (K) | 296 |
| *a*, *b*, *c* (Å) | 4.6032 (4), 6.9338 (8), 15.4421 (15) |
| $\alpha$, $\beta$, $\gamma$ (°) | 89.811 (4), 87.510 (3), 70.866 (3) |
| *V* (Å$^3$) | 465.18 (8) |
| *Z* | 1 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.23 |
| Crystal size (mm) | 0.16 × 0.14 × 0.10 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Sheldrick, 2003) |
| $T_{min}$, $T_{max}$ | 0.680, 0.744 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 16956, 4386, 3678 |
| $R_{int}$ | 0.039 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.668 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.041, 0.102, 1.11 |
| No. of reflections | 4386 |
| No. of parameters | 276 |
| No. of restraints | 3 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.22, −0.19 |
| Absolute structure | Flack (1983) |
| Absolute structure parameter | 0.05 (10) |

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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# full crystallographic data

*IUCrData* (2018). **3**, x180817 [https://doi.org/10.1107/S2414314618008179]

## *N*-(4-Chlorophenyl)-*N*′-{4-[(*Z*)-hydroxy(1-oxo-1,3-dihydro-2*H*-inden-2-ylidene)methyl]phenyl}urea

**Ísmail Çelik, Zeliha Atioğlu, Gamze Ordu, Hayreddin Gezegen and Mehmet Akkurt**

**_N_-(4-Chlorophenyl)-_N_′-{4-[(_Z_)-hydroxy(1-oxo-1,3-dihydro-2_H_-inden-2-ylidene)methyl]phenyl}urea**

*Crystal data*

$C_{23}H_{17}ClN_2O_3$
$M_r$ = 404.84
Triclinic, *P*1
Hall symbol: P 1
*a* = 4.6032 (4) Å
*b* = 6.9338 (8) Å
*c* = 15.4421 (15) Å
*α* = 89.811 (4)°
*β* = 87.510 (3)°
*γ* = 70.866 (3)°
*V* = 465.18 (8) Å$^3$
*Z* = 1
*F*(000) = 210
$D_x$ = 1.445 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9876 reflections
*θ* = 3.1–28.3°
*μ* = 0.23 mm$^{-1}$
*T* = 296 K
Block, yellow
0.16 × 0.14 × 0.10 mm

*Data collection*

Bruker APEXII CCD diffractometer
*φ* and *ω* scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min}$ = 0.680, $T_{max}$ = 0.744
16956 measured reflections
4386 independent reflections
3678 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039
$\theta_{max}$ = 28.4°, $\theta_{min}$ = 3.1°
*h* = −6→5
*k* = −9→9
*l* = −20→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.102
*S* = 1.11
4386 reflections
276 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 0.143P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.128 (16)
Absolute structure: Flack (1983)
Absolute structure parameter: 0.05 (10)

*Special details*

**Geometry**. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. The H-atoms of the OH and NH groups were freely refined [O—H = 0.89 (5) Å, N—H = 0.87 (6) and 0.81 (5) Å]. The C-bound H-atoms were placed at calculated positions, with C—H = 0.93 - 0.97 Å, and refined as riding on their carrier C-atom, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 | 0.5548 (8) | 0.8679 (5) | 0.1780 (2) | 0.0429 (8) |
| H1 | 0.5605 | 0.7338 | 0.1700 | 0.051* |
| C2 | 0.3778 (9) | 1.0201 (6) | 0.1255 (3) | 0.0515 (9) |
| H2 | 0.2630 | 0.9891 | 0.0828 | 0.062* |
| C3 | 0.3741 (9) | 1.2159 (5) | 0.1371 (2) | 0.0515 (10) |
| C4 | 0.5390 (10) | 1.2646 (5) | 0.1997 (3) | 0.0576 (11) |
| H4 | 0.5330 | 1.3990 | 0.2070 | 0.069* |
| C5 | 0.7158 (9) | 1.1128 (5) | 0.2523 (2) | 0.0491 (9) |
| H5 | 0.8301 | 1.1452 | 0.2948 | 0.059* |
| C6 | 0.7226 (6) | 0.9138 (4) | 0.2420 (2) | 0.0335 (6) |
| C7 | 0.8067 (6) | 0.6309 (4) | 0.3429 (2) | 0.0310 (6) |
| C8 | 0.9592 (6) | 0.3525 (4) | 0.4474 (2) | 0.0330 (7) |
| C9 | 0.7154 (7) | 0.4119 (4) | 0.5074 (2) | 0.0387 (7) |
| H9 | 0.5857 | 0.5468 | 0.5092 | 0.046* |
| C10 | 0.6618 (7) | 0.2726 (4) | 0.5648 (2) | 0.0389 (7) |
| H10 | 0.4958 | 0.3155 | 0.6048 | 0.047* |
| C11 | 0.8519 (7) | 0.0691 (4) | 0.5639 (2) | 0.0333 (6) |
| C12 | 1.0962 (7) | 0.0118 (5) | 0.5029 (2) | 0.0409 (8) |
| H12 | 1.2259 | −0.1231 | 0.5004 | 0.049* |
| C13 | 1.1506 (8) | 0.1517 (5) | 0.4456 (2) | 0.0425 (8) |
| H13 | 1.3170 | 0.1102 | 0.4057 | 0.051* |
| C14 | 0.8025 (7) | −0.0849 (4) | 0.6237 (2) | 0.0361 (7) |
| C15 | 0.5883 (7) | −0.0554 (5) | 0.6905 (2) | 0.0374 (7) |
| C16 | 0.3507 (7) | 0.1363 (5) | 0.7274 (2) | 0.0384 (7) |
| H16A | 0.4470 | 0.2324 | 0.7473 | 0.046* |
| H16B | 0.2022 | 0.2020 | 0.6848 | 0.046* |
| C17 | 0.2012 (8) | 0.0579 (5) | 0.8020 (2) | 0.0403 (7) |
| C18 | −0.0360 (9) | 0.1673 (6) | 0.8598 (2) | 0.0526 (9) |
| H18 | −0.1205 | 0.3085 | 0.8565 | 0.063* |
| C19 | −0.1423 (10) | 0.0608 (7) | 0.9221 (3) | 0.0630 (11) |
| H19 | −0.3000 | 0.1321 | 0.9612 | 0.076* |
| C20 | −0.0203 (10) | −0.1495 (7) | 0.9279 (3) | 0.0630 (11) |
| H20 | −0.0976 | −0.2170 | 0.9705 | 0.076* |

| | | | | |
|---|---|---|---|---|
| C21 | 0.2155 (10) | −0.2602 (6) | 0.8710 (3) | 0.0560 (10) |
| H21 | 0.2989 | −0.4015 | 0.8746 | 0.067* |
| C22 | 0.3231 (8) | −0.1528 (5) | 0.8084 (2) | 0.0423 (8) |
| C23 | 0.5676 (8) | −0.2277 (5) | 0.7414 (2) | 0.0424 (8) |
| Cl1 | 0.1535 (3) | 1.40938 (18) | 0.07167 (9) | 0.0914 (5) |
| N1 | 0.9113 (6) | 0.7605 (4) | 0.29524 (19) | 0.0409 (7) |
| N2 | 1.0222 (6) | 0.4939 (4) | 0.38897 (19) | 0.0394 (7) |
| O1 | 0.5366 (5) | 0.6352 (4) | 0.34347 (17) | 0.0434 (6) |
| O2 | 0.9969 (6) | −0.2732 (3) | 0.60665 (19) | 0.0527 (7) |
| O3 | 0.7349 (7) | −0.4103 (3) | 0.72891 (19) | 0.0589 (7) |
| H2N | 1.202 (10) | 0.487 (6) | 0.383 (3) | 0.052 (11)* |
| H1N | 1.100 (12) | 0.752 (7) | 0.303 (3) | 0.064 (13)* |
| H2O | 0.955 (12) | −0.353 (8) | 0.647 (3) | 0.083 (16)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.1031 (10) | 0.0650 (7) | 0.0752 (8) | 0.0144 (6) | −0.0048 (7) | 0.0354 (6) |
| O1 | 0.0243 (11) | 0.0494 (13) | 0.0607 (14) | −0.0172 (10) | −0.0089 (9) | 0.0211 (11) |
| O2 | 0.0614 (16) | 0.0255 (11) | 0.0601 (16) | −0.0012 (10) | 0.0120 (12) | 0.0047 (11) |
| O3 | 0.0753 (19) | 0.0300 (12) | 0.0624 (17) | −0.0063 (12) | 0.0066 (14) | 0.0116 (11) |
| N1 | 0.0239 (13) | 0.0464 (15) | 0.0561 (18) | −0.0162 (11) | −0.0072 (12) | 0.0212 (13) |
| N2 | 0.0199 (13) | 0.0440 (15) | 0.0556 (17) | −0.0122 (11) | −0.0050 (11) | 0.0180 (12) |
| C1 | 0.0452 (19) | 0.0348 (16) | 0.049 (2) | −0.0133 (14) | −0.0077 (15) | 0.0064 (14) |
| C2 | 0.055 (2) | 0.050 (2) | 0.047 (2) | −0.0142 (17) | −0.0103 (17) | 0.0118 (17) |
| C3 | 0.053 (2) | 0.0430 (18) | 0.044 (2) | 0.0024 (16) | 0.0071 (16) | 0.0151 (15) |
| C4 | 0.084 (3) | 0.0302 (17) | 0.056 (2) | −0.0173 (18) | 0.005 (2) | 0.0048 (15) |
| C5 | 0.063 (2) | 0.0416 (18) | 0.048 (2) | −0.0242 (16) | −0.0075 (17) | 0.0037 (15) |
| C6 | 0.0261 (14) | 0.0352 (15) | 0.0399 (16) | −0.0111 (11) | 0.0006 (12) | 0.0100 (12) |
| C7 | 0.0213 (14) | 0.0319 (14) | 0.0403 (16) | −0.0097 (11) | −0.0011 (11) | 0.0053 (12) |
| C8 | 0.0268 (15) | 0.0333 (15) | 0.0403 (17) | −0.0109 (12) | −0.0079 (12) | 0.0090 (12) |
| C9 | 0.0355 (17) | 0.0269 (14) | 0.0485 (19) | −0.0035 (12) | 0.0002 (14) | 0.0059 (13) |
| C10 | 0.0357 (17) | 0.0318 (16) | 0.0437 (19) | −0.0044 (13) | 0.0048 (13) | 0.0039 (13) |
| C11 | 0.0345 (15) | 0.0283 (14) | 0.0366 (16) | −0.0091 (11) | −0.0065 (12) | 0.0034 (12) |
| C12 | 0.0406 (18) | 0.0268 (15) | 0.048 (2) | −0.0009 (13) | −0.0018 (14) | 0.0046 (14) |
| C13 | 0.0330 (17) | 0.0430 (17) | 0.0455 (19) | −0.0051 (13) | 0.0036 (14) | 0.0067 (14) |
| C14 | 0.0390 (17) | 0.0256 (14) | 0.0403 (16) | −0.0056 (12) | −0.0057 (13) | 0.0033 (12) |
| C15 | 0.0420 (17) | 0.0308 (14) | 0.0383 (16) | −0.0100 (12) | −0.0059 (13) | 0.0090 (12) |
| C16 | 0.0404 (17) | 0.0332 (15) | 0.0377 (17) | −0.0060 (12) | −0.0061 (13) | 0.0074 (12) |
| C17 | 0.0397 (18) | 0.0443 (18) | 0.0345 (17) | −0.0100 (14) | −0.0056 (13) | 0.0082 (14) |
| C18 | 0.052 (2) | 0.053 (2) | 0.045 (2) | −0.0068 (17) | −0.0007 (16) | 0.0094 (17) |
| C19 | 0.056 (2) | 0.075 (3) | 0.047 (2) | −0.009 (2) | 0.0057 (18) | 0.014 (2) |
| C20 | 0.060 (3) | 0.073 (3) | 0.052 (2) | −0.018 (2) | 0.0037 (19) | 0.024 (2) |
| C21 | 0.059 (2) | 0.052 (2) | 0.055 (2) | −0.0158 (18) | −0.0078 (18) | 0.0229 (18) |
| C22 | 0.0459 (19) | 0.0421 (17) | 0.0383 (18) | −0.0126 (14) | −0.0092 (14) | 0.0112 (14) |
| C23 | 0.0503 (19) | 0.0352 (16) | 0.0406 (18) | −0.0120 (14) | −0.0072 (14) | 0.0078 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C3 | 1.743 (4) | C15—C16 | 1.512 (5) |
| O1—C7 | 1.234 (4) | C15—C23 | 1.455 (5) |
| O2—C14 | 1.338 (3) | C16—C17 | 1.506 (5) |
| O3—C23 | 1.258 (4) | C17—C18 | 1.393 (5) |
| N1—C6 | 1.418 (4) | C17—C22 | 1.388 (5) |
| N1—C7 | 1.353 (4) | C18—C19 | 1.379 (6) |
| N2—C7 | 1.353 (4) | C19—C20 | 1.384 (6) |
| N2—C8 | 1.420 (4) | C20—C21 | 1.384 (7) |
| O2—H2O | 0.89 (5) | C21—C22 | 1.389 (6) |
| C1—C2 | 1.387 (5) | C22—C23 | 1.458 (5) |
| C1—C6 | 1.380 (5) | C1—H1 | 0.9300 |
| N1—H1N | 0.87 (6) | C2—H2 | 0.9300 |
| N2—H2N | 0.81 (5) | C4—H4 | 0.9300 |
| C2—C3 | 1.365 (5) | C5—H5 | 0.9300 |
| C3—C4 | 1.363 (6) | C9—H9 | 0.9300 |
| C4—C5 | 1.386 (5) | C10—H10 | 0.9300 |
| C5—C6 | 1.380 (4) | C12—H12 | 0.9300 |
| C8—C9 | 1.377 (4) | C13—H13 | 0.9300 |
| C8—C13 | 1.382 (4) | C16—H16A | 0.9700 |
| C9—C10 | 1.382 (4) | C16—H16B | 0.9700 |
| C10—C11 | 1.395 (4) | C18—H18 | 0.9300 |
| C11—C14 | 1.476 (4) | C19—H19 | 0.9300 |
| C11—C12 | 1.388 (5) | C20—H20 | 0.9300 |
| C12—C13 | 1.386 (5) | C21—H21 | 0.9300 |
| C14—C15 | 1.363 (5) | | |
| | | | |
| C6—N1—C7 | 123.5 (3) | C17—C18—C19 | 118.3 (4) |
| C7—N2—C8 | 124.3 (3) | C18—C19—C20 | 121.7 (4) |
| C14—O2—H2O | 106 (3) | C19—C20—C21 | 120.7 (4) |
| C2—C1—C6 | 120.5 (3) | C20—C21—C22 | 117.6 (4) |
| C7—N1—H1N | 115 (3) | C17—C22—C21 | 122.0 (3) |
| C6—N1—H1N | 121 (3) | C17—C22—C23 | 108.4 (3) |
| C1—C2—C3 | 119.2 (4) | C21—C22—C23 | 129.6 (3) |
| C8—N2—H2N | 116 (3) | O3—C23—C22 | 126.3 (3) |
| C7—N2—H2N | 120 (3) | C15—C23—C22 | 108.7 (3) |
| Cl1—C3—C4 | 118.8 (3) | O3—C23—C15 | 125.0 (3) |
| C2—C3—C4 | 121.2 (3) | C2—C1—H1 | 120.00 |
| Cl1—C3—C2 | 120.0 (3) | C6—C1—H1 | 120.00 |
| C3—C4—C5 | 119.6 (3) | C1—C2—H2 | 120.00 |
| C4—C5—C6 | 120.2 (3) | C3—C2—H2 | 120.00 |
| N1—C6—C1 | 121.7 (3) | C3—C4—H4 | 120.00 |
| C1—C6—C5 | 119.1 (3) | C5—C4—H4 | 120.00 |
| N1—C6—C5 | 119.1 (3) | C4—C5—H5 | 120.00 |
| O1—C7—N2 | 122.5 (3) | C6—C5—H5 | 120.00 |
| O1—C7—N1 | 122.6 (3) | C8—C9—H9 | 120.00 |
| N1—C7—N2 | 114.9 (3) | C10—C9—H9 | 120.00 |

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| C9—C8—C13 | 119.1 (3) | C9—C10—H10 | 119.00 |
| N2—C8—C9 | 121.5 (2) | C11—C10—H10 | 119.00 |
| N2—C8—C13 | 119.4 (3) | C11—C12—H12 | 119.00 |
| C8—C9—C10 | 120.5 (3) | C13—C12—H12 | 119.00 |
| C9—C10—C11 | 121.3 (3) | C8—C13—H13 | 120.00 |
| C10—C11—C14 | 123.1 (3) | C12—C13—H13 | 120.00 |
| C12—C11—C14 | 119.5 (3) | C15—C16—H16A | 111.00 |
| C10—C11—C12 | 117.4 (3) | C15—C16—H16B | 111.00 |
| C11—C12—C13 | 121.3 (3) | C17—C16—H16A | 111.00 |
| C8—C13—C12 | 120.4 (3) | C17—C16—H16B | 111.00 |
| O2—C14—C11 | 112.9 (3) | H16A—C16—H16B | 109.00 |
| C11—C14—C15 | 127.9 (3) | C17—C18—H18 | 121.00 |
| O2—C14—C15 | 119.3 (3) | C19—C18—H18 | 121.00 |
| C14—C15—C23 | 120.2 (3) | C18—C19—H19 | 119.00 |
| C14—C15—C16 | 131.5 (3) | C20—C19—H19 | 119.00 |
| C16—C15—C23 | 108.2 (3) | C19—C20—H20 | 120.00 |
| C15—C16—C17 | 103.0 (3) | C21—C20—H20 | 120.00 |
| C16—C17—C18 | 128.7 (3) | C20—C21—H21 | 121.00 |
| C18—C17—C22 | 119.7 (3) | C22—C21—H21 | 121.00 |
| C16—C17—C22 | 111.6 (3) | | |

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| C7—N1—C6—C1 | −55.6 (4) | C12—C11—C14—C15 | 175.9 (3) |
| C7—N1—C6—C5 | 126.9 (3) | C11—C12—C13—C8 | −0.7 (5) |
| C6—N1—C7—O1 | 0.4 (5) | O2—C14—C15—C16 | 177.1 (3) |
| C6—N1—C7—N2 | 179.4 (3) | O2—C14—C15—C23 | −1.3 (5) |
| C7—N2—C8—C9 | −46.4 (4) | C11—C14—C15—C16 | −3.4 (6) |
| C7—N2—C8—C13 | 135.2 (3) | C11—C14—C15—C23 | 178.2 (3) |
| C8—N2—C7—N1 | 175.9 (3) | C14—C15—C16—C17 | −178.1 (4) |
| C8—N2—C7—O1 | −5.1 (5) | C23—C15—C16—C17 | 0.5 (4) |
| C6—C1—C2—C3 | 0.8 (6) | C14—C15—C23—O3 | −0.5 (6) |
| C2—C1—C6—N1 | −178.5 (3) | C14—C15—C23—C22 | 179.5 (3) |
| C2—C1—C6—C5 | −1.0 (5) | C16—C15—C23—O3 | −179.2 (3) |
| C1—C2—C3—C4 | −0.5 (6) | C16—C15—C23—C22 | 0.8 (4) |
| C1—C2—C3—Cl1 | 179.9 (3) | C15—C16—C17—C18 | −179.9 (4) |
| Cl1—C3—C4—C5 | −180.0 (3) | C15—C16—C17—C22 | −1.6 (4) |
| C2—C3—C4—C5 | 0.5 (7) | C16—C17—C18—C19 | 178.2 (4) |
| C3—C4—C5—C6 | −0.7 (6) | C22—C17—C18—C19 | 0.0 (6) |
| C4—C5—C6—N1 | 178.5 (3) | C16—C17—C22—C21 | −178.3 (4) |
| C4—C5—C6—C1 | 0.9 (5) | C16—C17—C22—C23 | 2.2 (4) |
| N2—C8—C9—C10 | −178.7 (3) | C18—C17—C22—C21 | 0.2 (6) |
| C13—C8—C9—C10 | −0.3 (5) | C18—C17—C22—C23 | −179.4 (3) |
| N2—C8—C13—C12 | 179.0 (3) | C17—C18—C19—C20 | −0.3 (7) |
| C9—C8—C13—C12 | 0.6 (5) | C18—C19—C20—C21 | 0.3 (7) |
| C8—C9—C10—C11 | 0.1 (5) | C19—C20—C21—C22 | −0.1 (7) |
| C9—C10—C11—C12 | −0.3 (5) | C20—C21—C22—C17 | −0.1 (6) |
| C9—C10—C11—C14 | −179.7 (3) | C20—C21—C22—C23 | 179.4 (4) |
| C10—C11—C12—C13 | 0.5 (5) | C17—C22—C23—O3 | 178.1 (4) |
| C14—C11—C12—C13 | −180.0 (3) | C17—C22—C23—C15 | −1.8 (4) |

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|---|---|---|---|
| C10—C11—C14—O2 | 174.9 (3) | C21—C22—C23—O3 | −1.4 (7) |
| C10—C11—C14—C15 | −4.7 (5) | C21—C22—C23—C15 | 178.7 (4) |
| C12—C11—C14—O2 | −4.6 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*O*···O3 | 0.89 (5) | 1.71 (5) | 2.543 (4) | 154 (5) |
| N1—H1*N*···O1$^{i}$ | 0.87 (6) | 2.03 (5) | 2.853 (4) | 158 (4) |
| N2—H2*N*···O1$^{i}$ | 0.81 (5) | 2.18 (5) | 2.904 (4) | 148 (4) |

Symmetry code: (i) *x*+1, *y*, *z*.