

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

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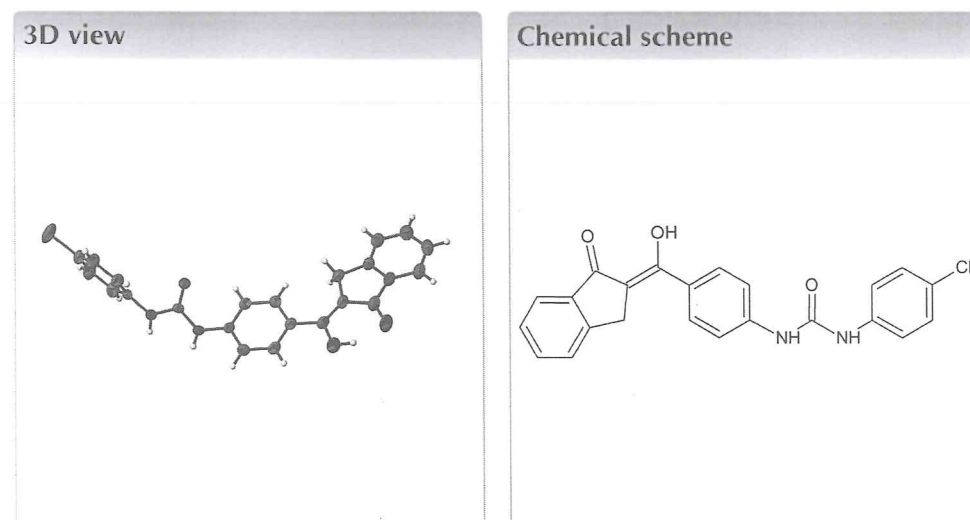
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**Keywords:** crystal structure; 2,3-dihydro-1*H*-indene ring system; N—H···O hydrogen bonds;  $\pi$ – $\pi$  stacking interaction.

**CCDC reference:** 1846924

**Structural data:** full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>23</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>3</sub>, 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*<sub>1</sub><sup>2</sup>(6) loops. Weak aromatic  $\pi$ – $\pi$  stacking [centroid–centroid distance = 3.656 (2) Å] is also observed.



## 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 now 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

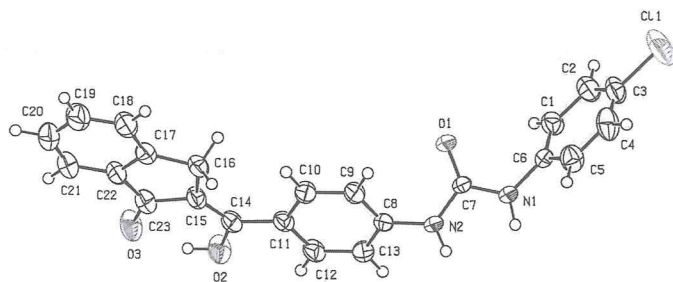
**Table 1**  
Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O2–H2O···O3	0.89 (5)	1.71 (5)	2.543 (4)	154 (5)
N1–H1N···O1 <sup>i</sup>	0.87 (6)	2.03 (5)	2.853 (4)	158 (4)
N2–H2N···O1 <sup>i</sup>	0.81 (5)	2.18 (5)	2.904 (4)	148 (4)

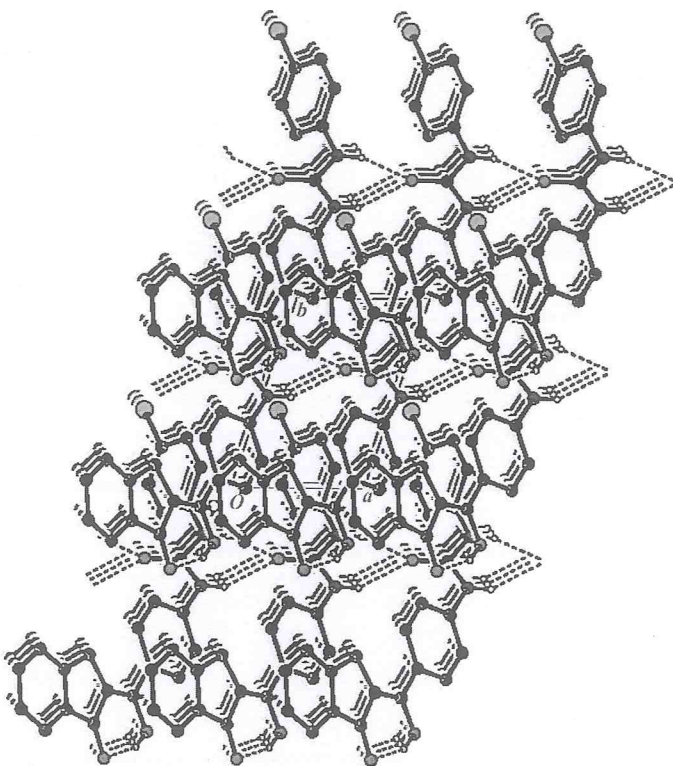
Symmetry code: (i)  $x + 1, y, z$ .

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  $^{\ast}[100]$  chains incorporating  $R_1^2(6)$  loops. In addition, weak aromatic  $\pi$ – $\pi$



**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.

stacking interactions are observed [ $Cg1 \cdots Cg4^i = 3.656 (2) \text{ \AA}$ ; *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),  $x + 1, y, z$ ].

### Synthesis and crystallization

For the synthesis 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, <i>P1</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	4.6032 (4), 6.9338 (8), 15.4421 (15)
$\alpha$ , $\beta$ , $\gamma$ (°)	89.811 (4), 87.510 (3), 70.866 (3)
<i>V</i> (Å <sup>3</sup> )	465.18 (8)
<i>Z</i>	1
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>−1</sup> )	0.23
Crystal size (mm)	0.16 × 0.14 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; 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
( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>−1</sup> )	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	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 <sup>−3</sup> )	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).

### Funding information

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### References

- Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, WI, Wisconsin, USA.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Gezegen, H., Hepokur, C., Tutar, U. & Ceylan, M. (2017). *Chem. Biodivers.* **14**, e1700223.
- Jiang, N., Bu, Y., Wang, Y., Nie, M., Zhang, D. & Zhai, X. (2016). *Molecules*, **21**, 1572–1583.
- Mague, J. T., Mohamed, S. K., Akkurt, M., Omran, O. A. & Albayati, M. R. (2015). *Acta Cryst.* **E71**, o88–o89.
- Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Sikka, P., Sahu, J. K., Mishra, A. K. & Hashim, S. R. (2015). *Med. Chem.* **5**, 479–483.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Yassine, H., Khouili, M., El Ammari, L., Saadi, M. & Ketatni, E. M. (2015). *Acta Cryst.* **E71**, o297–o298.

## full crystallographic data

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

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

*Crystal data*

C<sub>23</sub>H<sub>17</sub>ClN<sub>2</sub>O<sub>3</sub>

*M<sub>r</sub>* = 404.84

Triclinic, *P*1

Hall symbol: P 1

*a* = 4.6032 (4) Å

*b* = 6.9338 (8) Å

*c* = 15.4421 (15) Å

$\alpha$  = 89.811 (4)°

$\beta$  = 87.510 (3)°

$\gamma$  = 70.866 (3)°

*V* = 465.18 (8) Å<sup>3</sup>

*Z* = 1

*F*(000) = 210

*D<sub>x</sub>* = 1.445 Mg m<sup>-3</sup>

Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 9876 reflections

$\theta$  = 3.1–28.3°

$\mu$  = 0.23 mm<sup>-1</sup>

*T* = 296 K

Block, yellow

0.16 × 0.14 × 0.10 mm

*Data collection*

Bruker APEXII CCD

diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 2003)

*T<sub>min</sub>* = 0.680, *T<sub>max</sub>* = 0.744

16956 measured reflections

4386 independent reflections

3678 reflections with *I* > 2 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.039

$\theta_{\max}$  = 28.4°,  $\theta_{\min}$  = 3.1°

*h* = -6→5

*k* = -9→9

*l* = -20→20

*Refinement*

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$  = 0.041

*wR*(*F*<sup>2</sup>) = 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  $P = (F_o^2 + 2F_c^2)/3$

( $\Delta/\sigma$ )<sub>max</sub> < 0.001

$\Delta\rho_{\max}$  = 0.22 e Å<sup>-3</sup>

$\Delta\rho_{\min}$  = -0.19 e Å<sup>-3</sup>

Extinction correction: SHELXL2014

(Sheldrick, 2015),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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)
C11	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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	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, °)

C11—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)
C11—C3—C4	118.8 (3)	O3—C23—C15	125.0 (3)
C2—C3—C4	121.2 (3)	C2—C1—H1	120.00
C11—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

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)		
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—C11	179.9 (3)	C15—C16—C17—C18	-179.9 (4)
C11—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)		

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*Hydrogen-bond geometry (Å, °)*

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<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
O2—H2O···O3	0.89 (5)	1.71 (5)	2.543 (4)	154 (5)
N1—H1N···O1 <sup>i</sup>	0.87 (6)	2.03 (5)	2.853 (4)	158 (4)
N2—H2N···O1 <sup>i</sup>	0.81 (5)	2.18 (5)	2.904 (4)	148 (4)

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