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# 2-Amino-4-(2-chlorophenyl)-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile ethanol monosolvate

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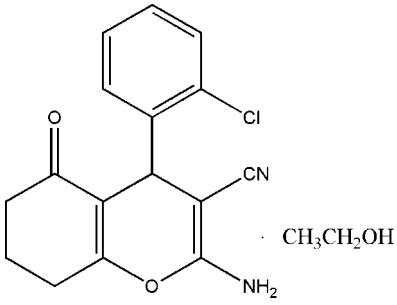
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.082; $wR$ factor = 0.230; data-to-parameter ratio = 13.7.

In the title compound, $C_{16}H_{13}ClN_2O_2\cdot C_2H_6O$, the fused cyclohexene and pyran rings adopt envelope and flattened boat conformations, respectively. In the crystal, N—H···O and O—H···O hydrogen bonds link the chromene and ethanol solvent molecules into infinite chains along the $c$ axis, and N—H···N hydrogen bonds link these chains into a three-dimensional framework. Weak C—H···$\pi$ interactions are also present.

## Related literature

For the background, see: Lokaj *et al.* (1990); Marco *et al.* (1993). For crystal structures similar to the title compound, see: Tu *et al.* (2001).




## Experimental

### Crystal data

$C_{16}H_{13}ClN_2O_2\cdot C_2H_6O$ $M_r$ = 346.80
Triclinic, $P\overline{1}$
$a$ = 8.7610 (8) Å
$b$ = 9.6281 (9) Å
$c$ = 10.7951 (11) Å
$\alpha$ = 76.878 (1)°
$\beta$ = 83.028 (2)°
$\gamma$ = 77.632 (1)°
$V$ = 863.69 (14) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.24 mm$^{-1}$
$T$ = 298 K
0.47 × 0.46 × 0.21 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.896, $T_{max}$ = 0.952
4606 measured reflections
3003 independent reflections
1428 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.230
$S$ = 0.90
3003 reflections
219 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

*Cg* is the centroid of the C1–C6 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···N1$^{i}$ | 0.86 | 2.19 | 3.037 (5) | 167 |
| N2—H2$B$···O3 | 0.86 | 1.99 | 2.851 (5) | 178 |
| O3—H3···O1$^{ii}$ | 0.82 | 1.97 | 2.765 (5) | 164 |
| C14—H14$B$···$Cg^{iii}$ | 0.97 | 2.96 | 3.704 (5) | 135 |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2312).

## References

Lokaj, J., Kettmann, V., Pavelčík, F., Ilavský, D. & Marchalín, Š. (1990). *Acta Cryst.* C**46**, 788–791.
Marco, J. L., Martin, G., Martin, N., Martinez-Grau, A., Seoane, C., Albert, A. & Cano, F. H. (1993). *Tetrahedron*, **49**, 7133–7144.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tu, S.-J., Deng, X., Fang, Y.-Y., Guo, Y.-M., Du, M. & Liu, X.-H. (2001). *Acta Cryst.* E**57**, o358–o359.

# supporting information

*Acta Cryst.* (2011). E**67**, o3099 [doi:10.1107/S1600536811043650]

# 2-Amino-4-(2-chlorophenyl)-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile ethanol monosolvate

**Yan Qiao, Lingqian Kong, Guifang Chen, Shengli Li and Zhiqing Gao**

## S1. Comment

The present investigation is a continuation of our work that includes syntheses and structural studies of polyfunctionalized substituted pyran derivatives, owing to their biological activities (Lokaj *et al.*, 1990; Marco *et al.*, 1993).We obtained the title compound, (I), and reported here its crystal structure in the paper.

In the crystal structure, it is observed that structure unit contains a substituted 5,6,7,8-tetrahydro-4H-chromene, a benzene ring and a ethanol solvate. The pyran ring adopts a sofa conformation, the dihedral angle between the (O2/C8-C11) plane and the C8/C7/C11 plane is 16.14 (4)°. Meanwhile, the (O2/C8-C11) plane forms an angle of 88.55 (13)° with the phenyl plane (C1-C6), which means that the pyran ring and the benzene ring is nearly perpendicular. In the crystal, the nitrile group is typical [N≡C = 1.148 (5)Å] and the carbonyl group also is reasonable [C═O =1.223 (6)Å].

Moreover, the plane (C10-C15) also adopts an chair configuration in the compound, and the dihedral angle between the (C10-C15) plane and the (C13-C15) plane is 46.19 (5)°.

In (I) (Fig. 1), the bond lengths and angles of the main molecule are normal and correspond to those observed in 2-amino-7,7-dimethyl-5-oxo-4-phenyl- 5,6,7,8-tetra-hydro-4H-chromene-3-carbonitrile (Tu *et al.*, 2001).

In the crystal structure, there exist typical intermolecular N-H···N, N—H···O, O—H···O hydrogen bonds and weak C-H···$\pi$ interactions (Table 1.). Intermolecular N-H···O and O—H···O hydrogen bonds link the molecules and ethanol solvent into infinite chain along c-axis and intermolecular hydrogen bonds link these chains forming three-dimensional framework.

## S2. Experimental

Malononitrile (5 mmol), 1,3-cyclohexanedione (5 mmol) and 2-chorobenzaldehyde (5 mmol) was dissolved in 20 ml DMF in a round-bottom flask. The mixture was warmed, with agitation, to 423 K over a period of 6 h. The resulting solution was cooled. Crystal of (I) suitable for X-ray diffraction analysis were obtained by recrystallized from ethanol.

## S3. Refinement

All H atoms were placed in geometrically idealized positions (N-H 0.86, O-H 0.82 and C-H 0.93-0.98 Å ) and treated as riding on their parent atoms, with $U_{iso}$(H) = 1.2-1.5$U_{eq}$(C) (C, O, N).

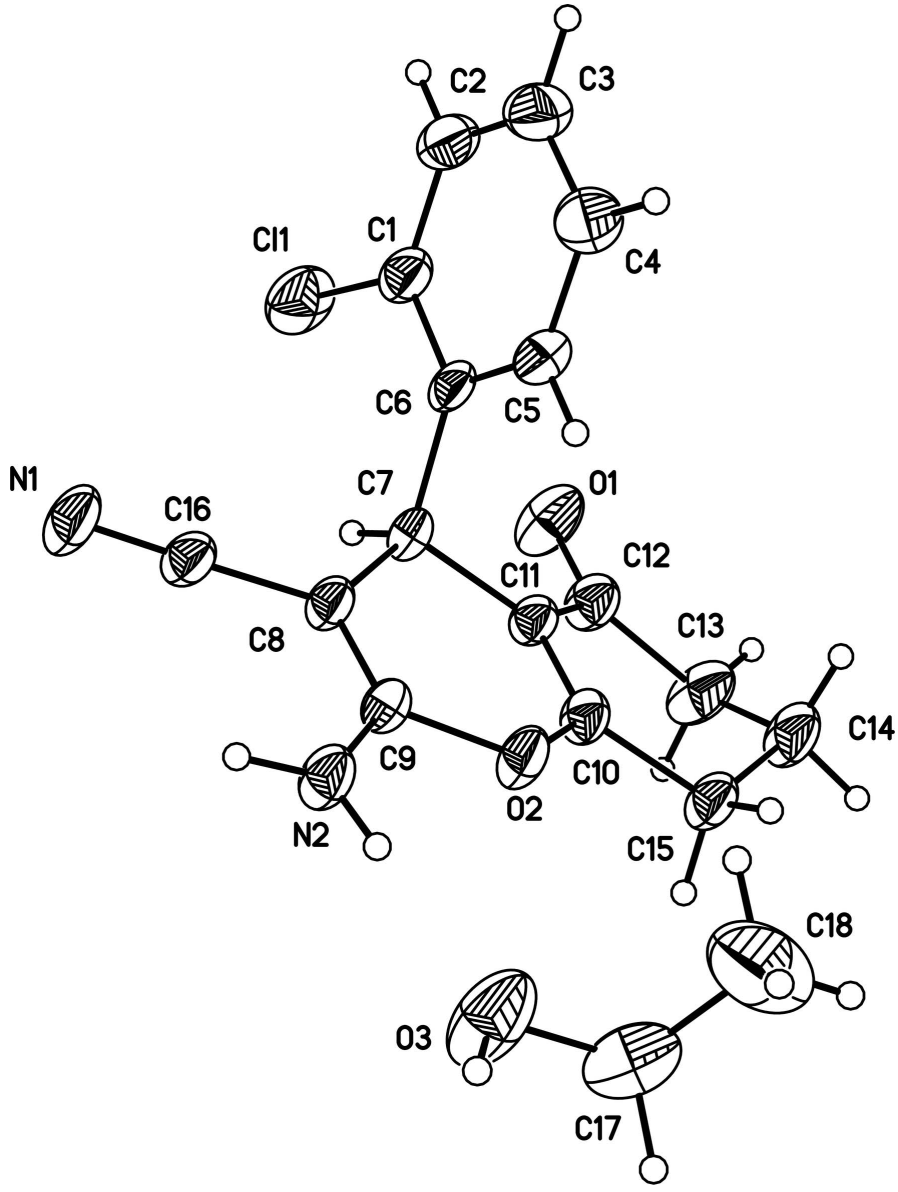


**Figure 1**

The title molecule with the atomic numbering scheme. The displacement ellipsoids are shown at the 30% probability level.

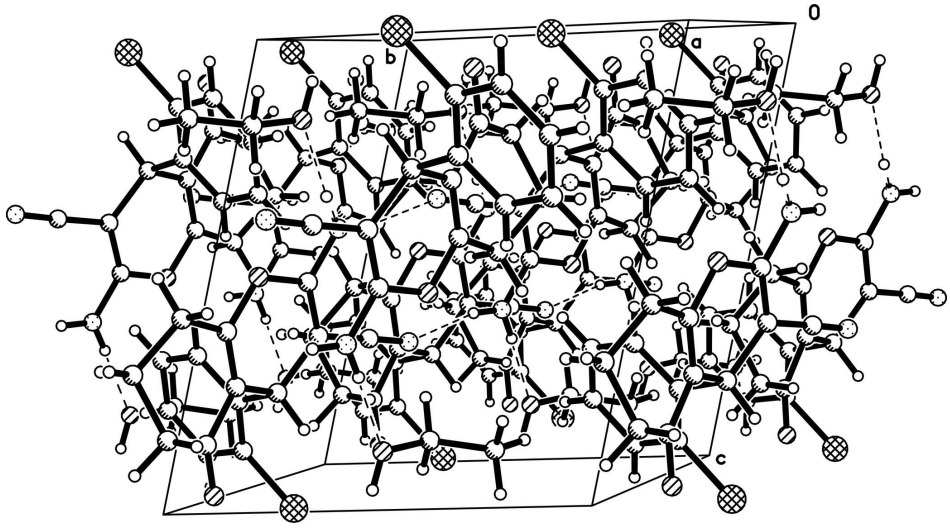


**Figure 2**

The packing of the title compound. N-H···N, N-H···O and O-H···O interactions are represented with dashed lines.

**2-Amino-4-(2-chlorophenyl)-5-oxo-5,6,7,8-tetrahydro- 4*H*-chromene-3-carbonitrile ethanol monosolvate**

*Crystal data*

$C_{16}H_{13}ClN_2O_2 \cdot C_2H_6O$
$M_r = 346.80$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.7610$ (8) Å
$b = 9.6281$ (9) Å
$c = 10.7951$ (11) Å
$\alpha = 76.878$ (1)°
$\beta = 83.028$ (2)°
$\gamma = 77.632$ (1)°
$V = 863.69$ (14) Å$^3$
$Z = 2$
$F(000) = 364$
$D_x = 1.334$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 821 reflections
$\theta = 2.6$–25.4°
$\mu = 0.24$ mm$^{-1}$
$T = 298$ K
Block, red
0.47 × 0.46 × 0.21 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.896$, $T_{max} = 0.952$
4606 measured reflections
3003 independent reflections
1428 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -10 \rightarrow 10$
$k = -9 \rightarrow 11$
$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.082$
$wR(F^2) = 0.230$
$S = 0.90$
3003 reflections
219 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.126P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.36$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.94359 (18) | 0.32844 (18) | 0.01378 (14) | 0.0853 (6) |
| N1 | 1.0042 (5) | 0.4987 (5) | 0.3508 (4) | 0.0694 (13) |
| N2 | 0.7142 (4) | 0.3876 (4) | 0.6036 (4) | 0.0543 (11) |
| H2A | 0.7912 | 0.4295 | 0.6051 | 0.065* |
| H2B | 0.6527 | 0.3694 | 0.6711 | 0.065* |
| O1 | 0.5581 (4) | 0.2859 (5) | 0.0845 (3) | 0.0796 (12) |
| O2 | 0.5602 (3) | 0.2879 (3) | 0.5179 (3) | 0.0531 (9) |
| O3 | 0.5099 (5) | 0.3347 (6) | 0.8285 (4) | 0.1065 (16) |
| H3 | 0.5180 | 0.3377 | 0.9026 | 0.160* |
| C1 | 0.9531 (5) | 0.1785 (6) | 0.1361 (5) | 0.0551 (13) |
| C2 | 1.0586 (6) | 0.0538 (7) | 0.1199 (6) | 0.0659 (15) |
| H2 | 1.1212 | 0.0522 | 0.0441 | 0.079* |
| C3 | 1.0716 (6) | −0.0672 (7) | 0.2153 (6) | 0.0736 (16) |
| H3A | 1.1434 | −0.1508 | 0.2047 | 0.088* |
| C4 | 0.9784 (6) | −0.0667 (6) | 0.3281 (6) | 0.0707 (16) |
| H4 | 0.9861 | −0.1494 | 0.3930 | 0.085* |
| C5 | 0.8745 (5) | 0.0572 (5) | 0.3432 (5) | 0.0532 (12) |
| H5 | 0.8139 | 0.0577 | 0.4201 | 0.064* |
| C6 | 0.8560 (4) | 0.1819 (5) | 0.2487 (4) | 0.0443 (11) |
| C7 | 0.7362 (4) | 0.3145 (5) | 0.2726 (4) | 0.0429 (11) |
| H7 | 0.7373 | 0.3918 | 0.1960 | 0.051* |
| C8 | 0.7721 (5) | 0.3698 (5) | 0.3836 (4) | 0.0437 (11) |
| C9 | 0.6906 (5) | 0.3513 (5) | 0.4982 (4) | 0.0437 (11) |
| C10 | 0.5007 (5) | 0.2644 (5) | 0.4148 (4) | 0.0454 (11) |
| C11 | 0.5740 (5) | 0.2806 (5) | 0.2992 (4) | 0.0433 (11) |
| C12 | 0.4933 (5) | 0.2721 (6) | 0.1923 (5) | 0.0561 (13) |
| C13 | 0.3260 (5) | 0.2516 (7) | 0.2181 (5) | 0.0745 (17) |
| H13A | 0.3012 | 0.2056 | 0.1539 | 0.089* |
| H13B | 0.2570 | 0.3459 | 0.2115 | 0.089* |
| C14 | 0.2971 (6) | 0.1595 (6) | 0.3488 (5) | 0.0670 (15) |
| H14A | 0.3567 | 0.0616 | 0.3523 | 0.080* |
| H14B | 0.1868 | 0.1544 | 0.3640 | 0.080* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.3445 (5) | 0.2227 (5) | 0.4516 (5) | 0.0541 (13) |
| H15A | 0.2668 | 0.3076 | 0.4644 | 0.065* |
| H15B | 0.3487 | 0.1515 | 0.5313 | 0.065* |
| C16 | 0.8995 (5) | 0.4412 (5) | 0.3669 (4) | 0.0489 (12) |
| C17 | 0.3742 (7) | 0.2814 (7) | 0.8216 (6) | 0.097 (2) |
| H17A | 0.3331 | 0.3234 | 0.7390 | 0.117* |
| H17B | 0.2949 | 0.3108 | 0.8865 | 0.117* |
| C18 | 0.4070 (11) | 0.1237 (8) | 0.8401 (7) | 0.136 (3) |
| H18A | 0.4878 | 0.0942 | 0.7776 | 0.204* |
| H18B | 0.3137 | 0.0910 | 0.8308 | 0.204* |
| H18C | 0.4412 | 0.0817 | 0.9240 | 0.204* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0840 (11) | 0.0960 (12) | 0.0676 (10) | −0.0272 (9) | 0.0204 (7) | −0.0043 (8) |
| N1 | 0.044 (2) | 0.100 (4) | 0.076 (3) | −0.036 (2) | 0.001 (2) | −0.025 (3) |
| N2 | 0.046 (2) | 0.078 (3) | 0.050 (3) | −0.029 (2) | −0.0001 (18) | −0.021 (2) |
| O1 | 0.060 (2) | 0.137 (4) | 0.052 (2) | −0.040 (2) | −0.0035 (18) | −0.023 (2) |
| O2 | 0.0437 (17) | 0.074 (2) | 0.050 (2) | −0.0305 (16) | 0.0028 (14) | −0.0154 (17) |
| O3 | 0.096 (3) | 0.183 (5) | 0.057 (3) | −0.070 (3) | 0.008 (2) | −0.025 (3) |
| C1 | 0.041 (3) | 0.071 (4) | 0.062 (3) | −0.020 (3) | 0.003 (2) | −0.026 (3) |
| C2 | 0.048 (3) | 0.086 (4) | 0.075 (4) | −0.018 (3) | 0.009 (3) | −0.041 (4) |
| C3 | 0.050 (3) | 0.074 (4) | 0.101 (5) | −0.003 (3) | −0.005 (3) | −0.036 (4) |
| C4 | 0.058 (3) | 0.069 (4) | 0.084 (4) | −0.008 (3) | −0.010 (3) | −0.014 (3) |
| C5 | 0.037 (3) | 0.061 (3) | 0.061 (3) | −0.012 (2) | 0.003 (2) | −0.014 (3) |
| C6 | 0.027 (2) | 0.059 (3) | 0.054 (3) | −0.018 (2) | 0.0017 (19) | −0.018 (2) |
| C7 | 0.031 (2) | 0.051 (3) | 0.049 (3) | −0.016 (2) | 0.0002 (18) | −0.008 (2) |
| C8 | 0.033 (2) | 0.056 (3) | 0.047 (3) | −0.017 (2) | −0.0002 (19) | −0.013 (2) |
| C9 | 0.031 (2) | 0.050 (3) | 0.053 (3) | −0.013 (2) | −0.0028 (19) | −0.012 (2) |
| C10 | 0.037 (2) | 0.054 (3) | 0.051 (3) | −0.017 (2) | −0.006 (2) | −0.015 (2) |
| C11 | 0.036 (2) | 0.054 (3) | 0.045 (3) | −0.015 (2) | 0.000 (2) | −0.017 (2) |
| C12 | 0.045 (3) | 0.074 (4) | 0.057 (3) | −0.019 (2) | −0.004 (2) | −0.020 (3) |
| C13 | 0.038 (3) | 0.125 (5) | 0.074 (4) | −0.027 (3) | −0.010 (2) | −0.037 (4) |
| C14 | 0.043 (3) | 0.091 (4) | 0.079 (4) | −0.032 (3) | −0.001 (2) | −0.026 (3) |
| C15 | 0.036 (3) | 0.068 (3) | 0.062 (3) | −0.020 (2) | 0.002 (2) | −0.015 (3) |
| C16 | 0.035 (2) | 0.064 (3) | 0.052 (3) | −0.014 (2) | −0.001 (2) | −0.018 (2) |
| C17 | 0.068 (4) | 0.131 (7) | 0.085 (5) | −0.004 (4) | 0.002 (3) | −0.021 (4) |
| C18 | 0.203 (10) | 0.088 (6) | 0.102 (6) | −0.006 (6) | 0.011 (6) | −0.020 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C1 | 1.716 (5) | C6—CG | 1.405 (4) |
| N1—C16 | 1.146 (5) | C6—C7 | 1.519 (6) |
| N2—C9 | 1.315 (5) | C7—C11 | 1.505 (5) |
| N2—H2A | 0.8600 | C7—C8 | 1.507 (6) |
| N2—H2B | 0.8600 | C7—H7 | 0.9800 |
| O1—C12 | 1.223 (5) | C8—C9 | 1.346 (6) |

| | | | |
|---|---|---|---|
| O2—C10 | 1.367 (5) | C8—C16 | 1.405 (6) |
| O2—C9 | 1.379 (5) | C10—C11 | 1.324 (6) |
| O3—C17 | 1.407 (7) | C10—C15 | 1.491 (6) |
| O3—H3 | 0.8200 | C11—C12 | 1.450 (6) |
| C1—CG | 1.373 (5) | C12—C13 | 1.505 (6) |
| C1—C2 | 1.381 (7) | C13—C14 | 1.511 (7) |
| C1—C6 | 1.399 (6) | C13—H13A | 0.9700 |
| C2—C3 | 1.363 (7) | C13—H13B | 0.9700 |
| C2—CG | 1.376 (5) | C14—C15 | 1.518 (6) |
| C2—H2 | 0.9300 | C14—H14A | 0.9700 |
| C3—CG | 1.376 (6) | C14—H14B | 0.9700 |
| C3—C4 | 1.382 (8) | C15—H15A | 0.9700 |
| C3—H3A | 0.9300 | C15—H15B | 0.9700 |
| C4—C5 | 1.366 (7) | C17—C18 | 1.455 (7) |
| C4—CG | 1.380 (6) | C17—H17A | 0.9700 |
| C4—H4 | 0.9300 | C17—H17B | 0.9700 |
| C5—CG | 1.359 (5) | C18—H18A | 0.9600 |
| C5—C6 | 1.381 (6) | C18—H18B | 0.9600 |
| C5—H5 | 0.9300 | C18—H18C | 0.9600 |

| | | | |
|---|---|---|---|
| C9—N2—H2A | 120.0 | C11—C10—C15 | 126.5 (4) |
| C9—N2—H2B | 120.0 | O2—C10—C15 | 110.5 (4) |
| H2A—N2—H2B | 120.0 | C10—C11—C12 | 119.2 (4) |
| C10—O2—C9 | 118.7 (3) | C10—C11—C7 | 122.6 (4) |
| C17—O3—H3 | 109.5 | C12—C11—C7 | 118.1 (4) |
| CG—C1—C2 | 60.0 (3) | O1—C12—C11 | 120.8 (4) |
| CG—C1—C6 | 60.9 (3) | O1—C12—C13 | 121.4 (4) |
| C2—C1—C6 | 120.8 (5) | C11—C12—C13 | 117.7 (4) |
| CG—C1—Cl1 | 178.0 (4) | C12—C13—C14 | 112.0 (4) |
| C2—C1—Cl1 | 118.1 (4) | C12—C13—H13A | 109.2 |
| C6—C1—Cl1 | 121.1 (4) | C14—C13—H13A | 109.2 |
| C3—C2—CG | 60.3 (3) | C12—C13—H13B | 109.2 |
| C3—C2—C1 | 120.0 (5) | C14—C13—H13B | 109.2 |
| CG—C2—C1 | 59.7 (3) | H13A—C13—H13B | 107.9 |
| C3—C2—H2 | 119.8 | C13—C14—C15 | 110.9 (4) |
| CG—C2—H2 | 179.7 | C13—C14—H14A | 109.5 |
| C1—C2—H2 | 120.1 | C15—C14—H14A | 109.5 |
| C2—C3—CG | 60.3 (3) | C13—C14—H14B | 109.5 |
| C2—C3—C4 | 120.4 (5) | C15—C14—H14B | 109.5 |
| CG—C3—C4 | 60.1 (3) | H14A—C14—H14B | 108.1 |
| C2—C3—H3A | 120.0 | C10—C15—C14 | 110.6 (4) |
| CG—C3—H3A | 179.6 | C10—C15—H15A | 109.5 |
| C4—C3—H3A | 119.6 | C14—C15—H15A | 109.5 |
| C5—C4—CG | 59.3 (3) | C10—C15—H15B | 109.5 |
| C5—C4—C3 | 119.1 (6) | C14—C15—H15B | 109.5 |
| CG—C4—C3 | 59.7 (4) | H15A—C15—H15B | 108.1 |
| C5—C4—H4 | 120.3 | N1—C16—C8 | 178.5 (5) |
| CG—C4—H4 | 179.5 | O3—C17—C18 | 111.4 (6) |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 120.6 | O3—C17—H17A | 109.3 |
| CG—C5—C4 | 60.9 (3) | C18—C17—H17A | 109.3 |
| CG—C5—C6 | 61.7 (3) | O3—C17—H17B | 109.3 |
| C4—C5—C6 | 122.6 (5) | C18—C17—H17B | 109.3 |
| CG—C5—H5 | 179.0 | H17A—C17—H17B | 108.0 |
| C4—C5—H5 | 118.7 | C17—C18—H18A | 109.5 |
| C6—C5—H5 | 118.8 | C17—C18—H18B | 109.5 |
| C5—C6—C1 | 117.0 (4) | H18A—C18—H18B | 109.5 |
| C5—C6—CG | 58.4 (3) | C17—C18—H18C | 109.5 |
| C1—C6—CG | 58.6 (3) | H18A—C18—H18C | 109.5 |
| C5—C6—C7 | 119.2 (4) | H18B—C18—H18C | 109.5 |
| C1—C6—C7 | 123.7 (4) | C5—CG—C1 | 120.4 (3) |
| CG—C6—C7 | 177.6 (4) | C5—CG—C3 | 120.0 (4) |
| C11—C7—C8 | 108.2 (3) | C1—CG—C3 | 119.7 (3) |
| C11—C7—C6 | 110.9 (3) | C5—CG—C2 | 179.3 (3) |
| C8—C7—C6 | 112.1 (3) | C1—CG—C2 | 60.3 (3) |
| C11—C7—H7 | 108.5 | C3—CG—C2 | 59.4 (3) |
| C8—C7—H7 | 108.5 | C5—CG—C4 | 59.8 (3) |
| C6—C7—H7 | 108.5 | C1—CG—C4 | 179.8 (3) |
| C9—C8—C16 | 118.6 (4) | C3—CG—C4 | 60.2 (3) |
| C9—C8—C7 | 123.3 (4) | C2—CG—C4 | 119.5 (3) |
| C16—C8—C7 | 118.0 (4) | C5—CG—C6 | 59.9 (3) |
| N2—C9—C8 | 129.3 (4) | C1—CG—C6 | 60.5 (3) |
| N2—C9—O2 | 109.7 (4) | C3—CG—C6 | 179.6 (3) |
| C8—C9—O2 | 121.0 (4) | C2—CG—C6 | 120.8 (3) |
| C11—C10—O2 | 123.0 (4) | C4—CG—C6 | 119.7 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···N1$^{i}$ | 0.86 | 2.19 | 3.037 (5) | 167 |
| N2—H2*B*···O3 | 0.86 | 1.99 | 2.851 (5) | 178 |
| O3—H3···O1$^{ii}$ | 0.82 | 1.97 | 2.765 (5) | 164 |
| C14—H14*B*···CG$^{iii}$ | 0.97 | 2.96 | 3.704 (5) | 135 |

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