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# (2*R*,3*R*)-1-(4-Chlorophenyl)-2-[(*S*)-2-nitro-1-phenylethyl]-3-phenylpentan-1-one

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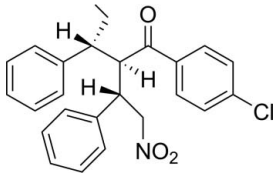
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.035; $wR$ factor = 0.099; data-to-parameter ratio = 15.8.

The title compound, $C_{25}H_{24}ClNO_3$, has three contiguous chiral centres. The absolute structure was determined by anomalous dispersion. The chlorobenzene ring is inclined to the two phenyl rings by 14.98 (9) and 59.05 (9)°. The two phenyl rings are inclined to one another by 49.51 (10)°. In the crystal, neighbouring molecules are linked *via* C—H···O hydrogen bonds, forming chains propagating along [010]. There is also a C—H···$\pi$ interaction present that leads to the formation of a three-dimensional network.

## Related literature

For the synthesis of the title compound, see: Xu *et al.* (2007). For the role of pyrrolidine motifs as organo-catalysts in asymmetric catalysis, see: Taylor & Jacobsen (2006) and for their role in bioactive molecules, see: Kawasaki *et al.* (2005).




## Experimental

### Crystal data

$C_{25}H_{24}ClNO_3$
$M_r$ = 421.90
Orthorhombic, $P2_12_12_1$
$a$ = 8.4700 (1) Å
$b$ = 13.1515 (2) Å
$c$ = 20.7060 (2) Å
$V$ = 2306.51 (5) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 1.66 mm$^{-1}$
$T$ = 293 K
0.42 × 0.36 × 0.30 mm

### Data collection

Gemini S Ultra Oxford Diffraction diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.542, $T_{max}$ = 0.635
22729 measured reflections
4292 independent reflections
4173 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
$S$ = 1.04
4292 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$
Absolute structure: Flack (1983), 1824 Friedel pairs
Flack parameter: −0.010 (13)

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C5—H5···O3$^{i}$ | 0.93 | 2.43 | 3.198 (5) | 140 |
| C12—H12···*CgA*$^{ii}$ | 0.93 | 2.82 | 3.691 (4) | 157 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2340).

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# supporting information

*Acta Cryst.* (2011). E**67**, o3495 [https://doi.org/10.1107/S1600536811050306]

## (2*R*,3*R*)-1-(4-Chlorophenyl)-2-[(*S*)-2-nitro-1-phenylethyl]-3-phenylpentan-1-one

**De-Long Duo, Cheng-Yan Ni and Qing-Song Wen**

### S1. Comment

Chiral pyrrolidines are readily obtained using the corresponding *γ*-nitro substituted carbonyl compounds (Xu *et al.*, 2007). Pyrrolidine motifs are important as synthetic intermediates as well as organo-catalysts in asymmetric catalysis (Taylor & Jacobsen, 2006) and they are also present in many bioactive molecules (Kawasaki *et al.*, 2005). *α*,*β*-unsaturated ketones react with nitro-olfine derivatives to produce *γ*-nitro ketones in good yields with high diastereoselectivities and enantioselectivities. The crystal structure of one such compound, the title optically pure compound, is described herein.

In the title molecule (Fig. 1), carbon atoms C8, C9 and C18 are three contiguous chiral centres, *R*, *R*, S, respectively. The chlorobenzene ring, A (C1—C6), and phenyl ring B (C10—C15), are inclined to one another by 14.98 (9)°. Phenyl ring C (C19—C24) make dihedral angles with rings A and B of 59.05 (9) and 49.51 (10)°, respectively.

In the crystal, neighbouring molecules are linked *via* C—H···O hydrogen bonds to form chains which propagate along the *b* axis direction (Tabe 1 and Fig. 2). There is also a C—H···*π* interaction (Table 1) present which leads to the formation of a three-dimensional network.

### S2. Experimental

The title compound was obtained by the procedure described by (Xu *et al.*, 2007). It was recrystallized from petroleun ether and ethyl acetate (*v*/*v* = 1:1), yielding colourless block-like crystals suitable for X-ray diffraction analysis.

### S3. Refinement

H atoms were placed in calculated positions with C—H = 0.93–0.98 Å, and refined in riding mode with $U_{iso}$(H) = 1.2$U_{eq}$(C).

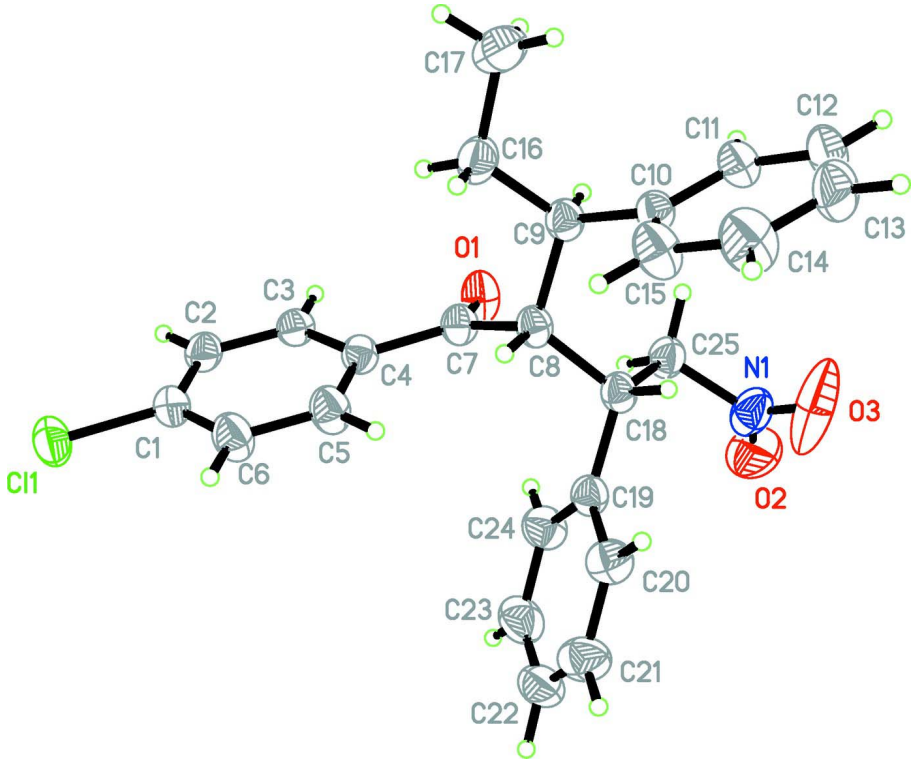


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering.

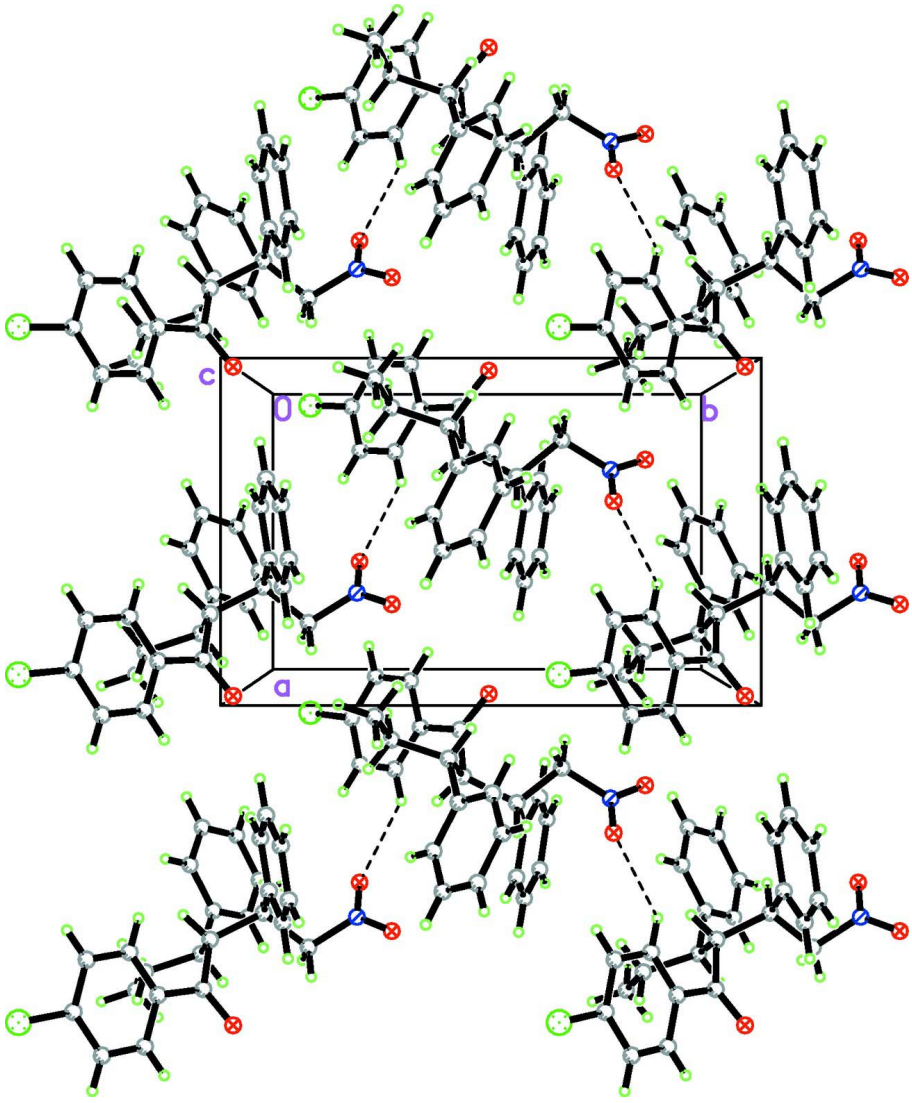


**Figure 2**

Crystal packing of the title compound, viewed along the *c* axis, showing the neighbouring molecules linked *via* C—H···O interactions (dashed lines), which generate chains propagating along the *b* axis direction.

**(2*R*,3*R*)-1-(4-Chlorophenyl)-2-[(*S*)-2-nitro-1-phenylethyl]- 3-phenylpentan-1-one**

*Crystal data*

$C_{25}H_{24}ClNO_3$
$M_r = 421.90$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.4700\ (1)$ Å
$b = 13.1515\ (2)$ Å
$c = 20.7060\ (2)$ Å
$V = 2306.51\ (5)$ Å$^3$
$Z = 4$
$F(000) = 888$
$D_x = 1.215$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 16354 reflections
$\theta = 3.4$–$69.8°$
$\mu = 1.66$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.42 × 0.36 × 0.30 mm

*Data collection*

Gemini S Ultra Oxford Diffraction diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 15.9149 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.542, $T_{max}$ = 0.635
22729 measured reflections
4292 independent reflections
4173 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019
$\theta_{max}$ = 69.9°, $\theta_{min}$ = 4.0°
$h$ = −10→10
$k$ = −15→16
$l$ = −21→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
$S$ = 1.04
4292 reflections
272 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.1848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$
Absolute structure: Flack (1983), 1824 Friedel pairs
Absolute structure parameter: −0.010 (13)

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.58917 (6) | 0.37368 (4) | 0.50249 (2) | 0.08473 (17) |
| O1 | 0.50133 (14) | 0.00173 (10) | 0.28825 (7) | 0.0700 (3) |
| O2 | 0.7782 (3) | −0.30696 (14) | 0.25735 (12) | 0.1277 (8) |
| O3 | 0.9069 (3) | −0.23945 (18) | 0.18103 (18) | 0.1769 (14) |
| N1 | 0.8118 (2) | −0.23648 (13) | 0.22259 (12) | 0.0826 (5) |
| C1 | 0.5978 (2) | 0.28418 (13) | 0.44074 (8) | 0.0595 (4) |
| C2 | 0.46287 (19) | 0.23354 (13) | 0.42310 (7) | 0.0565 (4) |
| H2 | 0.3673 | 0.2482 | 0.4431 | 0.068* |
| C3 | 0.47066 (18) | 0.16045 (12) | 0.37513 (7) | 0.0509 (3) |
| H3 | 0.3801 | 0.1251 | 0.3634 | 0.061* |
| C4 | 0.61302 (18) | 0.13951 (11) | 0.34438 (7) | 0.0495 (3) |
| C5 | 0.7473 (2) | 0.19166 (15) | 0.36286 (9) | 0.0646 (4) |
| H5 | 0.8430 | 0.1778 | 0.3427 | 0.078* |
| C6 | 0.7404 (2) | 0.26467 (16) | 0.41126 (9) | 0.0697 (5) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.8308 | 0.2999 | 0.4236 | 0.084* |
| C7 | 0.61293 (18) | 0.05938 (12) | 0.29275 (7) | 0.0519 (3) |
| C8 | 0.74862 (17) | 0.05223 (12) | 0.24430 (7) | 0.0499 (3) |
| H8 | 0.8271 | 0.1037 | 0.2561 | 0.060* |
| C9 | 0.68287 (19) | 0.08030 (12) | 0.17641 (8) | 0.0544 (3) |
| H9 | 0.5912 | 0.0368 | 0.1681 | 0.065* |
| C10 | 0.80251 (19) | 0.06096 (12) | 0.12331 (7) | 0.0528 (3) |
| C11 | 0.7672 (2) | −0.00341 (15) | 0.07273 (8) | 0.0664 (4) |
| H11 | 0.6694 | −0.0355 | 0.0720 | 0.080* |
| C12 | 0.8725 (3) | −0.02151 (18) | 0.02330 (10) | 0.0846 (6) |
| H12 | 0.8454 | −0.0651 | −0.0103 | 0.102* |
| C13 | 1.0170 (3) | 0.0248 (2) | 0.02388 (11) | 0.0923 (7) |
| H13 | 1.0893 | 0.0123 | −0.0090 | 0.111* |
| C14 | 1.0545 (3) | 0.0903 (2) | 0.07361 (12) | 0.0973 (7) |
| H14 | 1.1523 | 0.1224 | 0.0740 | 0.117* |
| C15 | 0.9477 (2) | 0.10866 (18) | 0.12305 (10) | 0.0763 (5) |
| H15 | 0.9740 | 0.1533 | 0.1562 | 0.092* |
| C16 | 0.6259 (3) | 0.19137 (16) | 0.17528 (9) | 0.0745 (5) |
| H16A | 0.5516 | 0.2017 | 0.2104 | 0.089* |
| H16B | 0.7154 | 0.2359 | 0.1826 | 0.089* |
| C17 | 0.5474 (3) | 0.2207 (2) | 0.11228 (12) | 0.0983 (7) |
| H17A | 0.4587 | 0.1769 | 0.1046 | 0.148* |
| H17B | 0.6218 | 0.2139 | 0.0776 | 0.148* |
| H17C | 0.5119 | 0.2899 | 0.1147 | 0.148* |
| C18 | 0.83087 (17) | −0.05335 (12) | 0.24718 (7) | 0.0512 (3) |
| H18 | 0.9132 | −0.0522 | 0.2139 | 0.061* |
| C19 | 0.91484 (19) | −0.07057 (11) | 0.31084 (7) | 0.0529 (3) |
| C20 | 1.0760 (2) | −0.05423 (14) | 0.31501 (9) | 0.0652 (4) |
| H20 | 1.1310 | −0.0316 | 0.2789 | 0.078* |
| C21 | 1.1568 (3) | −0.07107 (16) | 0.37241 (12) | 0.0809 (6) |
| H21 | 1.2651 | −0.0595 | 0.3743 | 0.097* |
| C22 | 1.0794 (3) | −0.10408 (16) | 0.42545 (10) | 0.0813 (6) |
| H22 | 1.1345 | −0.1166 | 0.4635 | 0.098* |
| C23 | 0.9185 (3) | −0.11912 (17) | 0.42302 (9) | 0.0825 (6) |
| H23 | 0.8646 | −0.1406 | 0.4597 | 0.099* |
| C24 | 0.8368 (2) | −0.10225 (17) | 0.36589 (9) | 0.0702 (5) |
| H24 | 0.7282 | −0.1124 | 0.3647 | 0.084* |
| C25 | 0.7198 (2) | −0.14079 (12) | 0.22928 (9) | 0.0595 (4) |
| H25A | 0.6401 | −0.1489 | 0.2626 | 0.071* |
| H25B | 0.6667 | −0.1255 | 0.1889 | 0.071* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0818 (3) | 0.0920 (3) | 0.0804 (3) | 0.0158 (3) | −0.0070 (2) | −0.0388 (2) |
| O1 | 0.0573 (6) | 0.0679 (7) | 0.0848 (8) | −0.0145 (6) | 0.0197 (6) | −0.0212 (6) |
| O2 | 0.173 (2) | 0.0687 (10) | 0.1411 (17) | 0.0274 (12) | −0.0380 (16) | 0.0015 (11) |
| O3 | 0.1117 (16) | 0.1051 (15) | 0.314 (4) | 0.0056 (12) | 0.093 (2) | −0.073 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0698 (10) | 0.0618 (10) | 0.1162 (14) | 0.0089 (8) | −0.0152 (10) | −0.0261 (10) |
| C1 | 0.0637 (9) | 0.0612 (9) | 0.0537 (8) | 0.0092 (8) | −0.0010 (7) | −0.0099 (7) |
| C2 | 0.0540 (8) | 0.0620 (8) | 0.0536 (8) | 0.0105 (7) | 0.0070 (6) | −0.0017 (7) |
| C3 | 0.0480 (7) | 0.0555 (8) | 0.0493 (7) | 0.0025 (6) | 0.0041 (6) | 0.0031 (6) |
| C4 | 0.0502 (7) | 0.0518 (7) | 0.0465 (7) | 0.0006 (6) | 0.0057 (6) | −0.0005 (6) |
| C5 | 0.0518 (8) | 0.0776 (11) | 0.0645 (9) | −0.0060 (8) | 0.0100 (7) | −0.0164 (8) |
| C6 | 0.0586 (9) | 0.0806 (12) | 0.0698 (10) | −0.0073 (9) | 0.0011 (8) | −0.0215 (9) |
| C7 | 0.0490 (7) | 0.0529 (7) | 0.0539 (7) | −0.0023 (6) | 0.0069 (6) | −0.0027 (6) |
| C8 | 0.0467 (7) | 0.0538 (7) | 0.0493 (7) | −0.0039 (6) | 0.0071 (6) | −0.0063 (6) |
| C9 | 0.0505 (7) | 0.0588 (8) | 0.0540 (8) | 0.0016 (6) | 0.0059 (6) | −0.0044 (7) |
| C10 | 0.0554 (8) | 0.0547 (8) | 0.0481 (7) | 0.0027 (7) | 0.0048 (6) | −0.0021 (6) |
| C11 | 0.0731 (10) | 0.0700 (10) | 0.0561 (9) | −0.0023 (9) | −0.0004 (8) | −0.0106 (8) |
| C12 | 0.1079 (17) | 0.0870 (13) | 0.0590 (10) | 0.0122 (12) | 0.0094 (11) | −0.0191 (9) |
| C13 | 0.0968 (16) | 0.1098 (17) | 0.0703 (12) | 0.0169 (13) | 0.0332 (12) | −0.0050 (12) |
| C14 | 0.0749 (13) | 0.129 (2) | 0.0881 (14) | −0.0200 (13) | 0.0292 (11) | −0.0019 (14) |
| C15 | 0.0699 (10) | 0.0919 (14) | 0.0670 (10) | −0.0222 (10) | 0.0142 (9) | −0.0140 (10) |
| C16 | 0.0882 (13) | 0.0710 (11) | 0.0642 (10) | 0.0241 (10) | 0.0141 (9) | 0.0008 (8) |
| C17 | 0.1010 (17) | 0.1026 (17) | 0.0914 (15) | 0.0363 (14) | −0.0009 (13) | 0.0153 (13) |
| C18 | 0.0470 (7) | 0.0555 (8) | 0.0511 (7) | −0.0004 (6) | 0.0059 (6) | −0.0062 (6) |
| C19 | 0.0539 (8) | 0.0496 (7) | 0.0553 (8) | −0.0017 (6) | 0.0004 (6) | −0.0061 (6) |
| C20 | 0.0575 (9) | 0.0636 (9) | 0.0745 (10) | −0.0104 (8) | −0.0033 (8) | 0.0006 (8) |
| C21 | 0.0746 (12) | 0.0727 (12) | 0.0954 (15) | −0.0100 (10) | −0.0249 (11) | −0.0021 (11) |
| C22 | 0.1026 (15) | 0.0691 (11) | 0.0723 (11) | 0.0028 (11) | −0.0278 (11) | −0.0100 (9) |
| C23 | 0.1092 (16) | 0.0836 (13) | 0.0548 (9) | 0.0021 (13) | 0.0032 (10) | 0.0032 (9) |
| C24 | 0.0649 (10) | 0.0858 (12) | 0.0597 (9) | −0.0035 (9) | 0.0063 (8) | 0.0015 (9) |
| C25 | 0.0562 (8) | 0.0541 (8) | 0.0680 (9) | 0.0028 (7) | −0.0036 (7) | −0.0117 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C1 | 1.7393 (15) | C12—H12 | 0.9300 |
| O1—C7 | 1.2153 (19) | C13—C14 | 1.379 (4) |
| O2—N1 | 1.208 (3) | C13—H13 | 0.9300 |
| O3—N1 | 1.180 (3) | C14—C15 | 1.387 (3) |
| N1—C25 | 1.487 (2) | C14—H14 | 0.9300 |
| C1—C2 | 1.372 (3) | C15—H15 | 0.9300 |
| C1—C6 | 1.378 (3) | C16—C17 | 1.514 (3) |
| C2—C3 | 1.384 (2) | C16—H16A | 0.9700 |
| C2—H2 | 0.9300 | C16—H16B | 0.9700 |
| C3—C4 | 1.391 (2) | C17—H17A | 0.9600 |
| C3—H3 | 0.9300 | C17—H17B | 0.9600 |
| C4—C5 | 1.382 (2) | C17—H17C | 0.9600 |
| C4—C7 | 1.501 (2) | C18—C19 | 1.515 (2) |
| C5—C6 | 1.389 (3) | C18—C25 | 1.531 (2) |
| C5—H5 | 0.9300 | C18—H18 | 0.9800 |
| C6—H6 | 0.9300 | C19—C24 | 1.382 (2) |
| C7—C8 | 1.5285 (19) | C19—C20 | 1.385 (2) |
| C8—C18 | 1.555 (2) | C20—C21 | 1.389 (3) |
| C8—C9 | 1.556 (2) | C20—H20 | 0.9300 |

| | | | |
|---|---|---|---|
| C8—H8 | 0.9800 | C21—C22 | 1.351 (3) |
| C9—C10 | 1.517 (2) | C21—H21 | 0.9300 |
| C9—C16 | 1.539 (2) | C22—C23 | 1.378 (4) |
| C9—H9 | 0.9800 | C22—H22 | 0.9300 |
| C10—C11 | 1.379 (2) | C23—C24 | 1.388 (3) |
| C10—C15 | 1.381 (2) | C23—H23 | 0.9300 |
| C11—C12 | 1.378 (3) | C24—H24 | 0.9300 |
| C11—H11 | 0.9300 | C25—H25A | 0.9700 |
| C12—C13 | 1.367 (4) | C25—H25B | 0.9700 |

| | | | |
|---|---|---|---|
| O3—N1—O2 | 124.8 (2) | C13—C14—C15 | 120.6 (2) |
| O3—N1—C25 | 117.0 (2) | C13—C14—H14 | 119.7 |
| O2—N1—C25 | 118.1 (2) | C15—C14—H14 | 119.7 |
| C2—C1—C6 | 121.45 (14) | C10—C15—C14 | 120.29 (19) |
| C2—C1—Cl1 | 119.29 (12) | C10—C15—H15 | 119.9 |
| C6—C1—Cl1 | 119.25 (14) | C14—C15—H15 | 119.9 |
| C1—C2—C3 | 119.24 (14) | C17—C16—C9 | 113.12 (18) |
| C1—C2—H2 | 120.4 | C17—C16—H16A | 109.0 |
| C3—C2—H2 | 120.4 | C9—C16—H16A | 109.0 |
| C2—C3—C4 | 120.49 (14) | C17—C16—H16B | 109.0 |
| C2—C3—H3 | 119.8 | C9—C16—H16B | 109.0 |
| C4—C3—H3 | 119.8 | H16A—C16—H16B | 107.8 |
| C5—C4—C3 | 119.23 (13) | C16—C17—H17A | 109.5 |
| C5—C4—C7 | 123.09 (13) | C16—C17—H17B | 109.5 |
| C3—C4—C7 | 117.67 (13) | H17A—C17—H17B | 109.5 |
| C4—C5—C6 | 120.54 (16) | C16—C17—H17C | 109.5 |
| C4—C5—H5 | 119.7 | H17A—C17—H17C | 109.5 |
| C6—C5—H5 | 119.7 | H17B—C17—H17C | 109.5 |
| C1—C6—C5 | 119.03 (17) | C19—C18—C25 | 112.75 (14) |
| C1—C6—H6 | 120.5 | C19—C18—C8 | 112.17 (12) |
| C5—C6—H6 | 120.5 | C25—C18—C8 | 112.71 (13) |
| O1—C7—C4 | 119.54 (13) | C19—C18—H18 | 106.2 |
| O1—C7—C8 | 119.74 (13) | C25—C18—H18 | 106.2 |
| C4—C7—C8 | 120.68 (13) | C8—C18—H18 | 106.2 |
| C7—C8—C18 | 111.51 (12) | C24—C19—C20 | 117.82 (16) |
| C7—C8—C9 | 108.01 (12) | C24—C19—C18 | 122.57 (15) |
| C18—C8—C9 | 114.01 (12) | C20—C19—C18 | 119.61 (15) |
| C7—C8—H8 | 107.7 | C19—C20—C21 | 120.96 (19) |
| C18—C8—H8 | 107.7 | C19—C20—H20 | 119.5 |
| C9—C8—H8 | 107.7 | C21—C20—H20 | 119.5 |
| C10—C9—C16 | 110.97 (14) | C22—C21—C20 | 120.5 (2) |
| C10—C9—C8 | 112.08 (12) | C22—C21—H21 | 119.7 |
| C16—C9—C8 | 110.56 (14) | C20—C21—H21 | 119.7 |
| C10—C9—H9 | 107.7 | C21—C22—C23 | 119.76 (19) |
| C16—C9—H9 | 107.7 | C21—C22—H22 | 120.1 |
| C8—C9—H9 | 107.7 | C23—C22—H22 | 120.1 |
| C11—C10—C15 | 117.99 (16) | C22—C23—C24 | 120.1 (2) |
| C11—C10—C9 | 120.55 (15) | C22—C23—H23 | 120.0 |

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| C15—C10—C9 | 121.44 (15) | C24—C23—H23 | 120.0 |
| C12—C11—C10 | 121.95 (19) | C19—C24—C23 | 120.83 (19) |
| C12—C11—H11 | 119.0 | C19—C24—H24 | 119.6 |
| C10—C11—H11 | 119.0 | C23—C24—H24 | 119.6 |
| C13—C12—C11 | 119.7 (2) | N1—C25—C18 | 109.64 (14) |
| C13—C12—H12 | 120.1 | N1—C25—H25A | 109.7 |
| C11—C12—H12 | 120.1 | C18—C25—H25A | 109.7 |
| C12—C13—C14 | 119.41 (19) | N1—C25—H25B | 109.7 |
| C12—C13—H13 | 120.3 | C18—C25—H25B | 109.7 |
| C14—C13—H13 | 120.3 | H25A—C25—H25B | 108.2 |

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| C6—C1—C2—C3 | 0.7 (3) | C10—C11—C12—C13 | 0.3 (4) |
| Cl1—C1—C2—C3 | −178.32 (12) | C11—C12—C13—C14 | −0.9 (4) |
| C1—C2—C3—C4 | −1.0 (2) | C12—C13—C14—C15 | 0.5 (4) |
| C2—C3—C4—C5 | 0.8 (2) | C11—C10—C15—C14 | −1.0 (3) |
| C2—C3—C4—C7 | −179.95 (14) | C9—C10—C15—C14 | −179.4 (2) |
| C3—C4—C5—C6 | −0.4 (3) | C13—C14—C15—C10 | 0.4 (4) |
| C7—C4—C5—C6 | −179.60 (17) | C10—C9—C16—C17 | 60.0 (2) |
| C2—C1—C6—C5 | −0.3 (3) | C8—C9—C16—C17 | −174.97 (18) |
| Cl1—C1—C6—C5 | 178.72 (16) | C7—C8—C18—C19 | −66.22 (16) |
| C4—C5—C6—C1 | 0.2 (3) | C9—C8—C18—C19 | 171.13 (12) |
| C5—C4—C7—O1 | 164.28 (18) | C7—C8—C18—C25 | 62.33 (17) |
| C3—C4—C7—O1 | −14.9 (2) | C9—C8—C18—C25 | −60.31 (17) |
| C5—C4—C7—C8 | −18.1 (2) | C25—C18—C19—C24 | −47.1 (2) |
| C3—C4—C7—C8 | 162.74 (14) | C8—C18—C19—C24 | 81.41 (19) |
| O1—C7—C8—C18 | −61.3 (2) | C25—C18—C19—C20 | 132.96 (16) |
| C4—C7—C8—C18 | 121.03 (15) | C8—C18—C19—C20 | −98.51 (16) |
| O1—C7—C8—C9 | 64.69 (19) | C24—C19—C20—C21 | 1.2 (3) |
| C4—C7—C8—C9 | −112.95 (15) | C18—C19—C20—C21 | −178.86 (17) |
| C7—C8—C9—C10 | −171.81 (13) | C19—C20—C21—C22 | 0.1 (3) |
| C18—C8—C9—C10 | −47.28 (18) | C20—C21—C22—C23 | −1.4 (3) |
| C7—C8—C9—C16 | 63.81 (17) | C21—C22—C23—C24 | 1.2 (3) |
| C18—C8—C9—C16 | −171.65 (14) | C20—C19—C24—C23 | −1.4 (3) |
| C16—C9—C10—C11 | −113.53 (19) | C18—C19—C24—C23 | 178.72 (17) |
| C8—C9—C10—C11 | 122.32 (17) | C22—C23—C24—C19 | 0.2 (3) |
| C16—C9—C10—C15 | 64.8 (2) | O3—N1—C25—C18 | −63.7 (3) |
| C8—C9—C10—C15 | −59.3 (2) | O2—N1—C25—C18 | 120.2 (2) |
| C15—C10—C11—C12 | 0.7 (3) | C19—C18—C25—N1 | −60.96 (19) |
| C9—C10—C11—C12 | 179.12 (18) | C8—C18—C25—N1 | 170.79 (16) |

*Hydrogen-bond geometry (Å, º)*

CgA is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5···O3$^{i}$ | 0.93 | 2.43 | 3.198 (5) | 140 |
| C12—H12···CgA$^{ii}$ | 0.93 | 2.82 | 3.691 (4) | 157 |

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