Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (2*SR*,3*RS*)-Benzyl[4-chloro-1-(4-chlorophenyl)-1-methoxycarbonyl-2-butyl]-ammonium chloride

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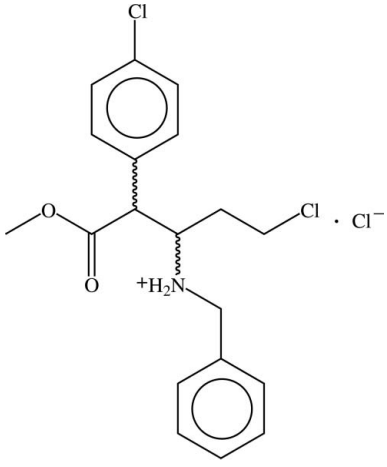
Received 22 September 2008; accepted 24 September 2008

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.047; $wR$ factor = 0.159; data-to-parameter ratio = 19.5.

In the racemic hydrochloride salt of the title ester, $C_{19}H_{22}Cl_2NO_2^+\cdot Cl^-$, the pentanoic acid chain shows a mixture of *trans* and *gauche* orientations to give an overall helical conformation. The dihedral angle between the two aromatic rings is 26.11 (10)°. The charged secondary amine function participates in two N—H···Cl hydrogen bonds.

## Related literature

For a related structure, see: Froimowitz *et al.* (1998).




## Experimental

### Crystal data

$C_{19}H_{22}Cl_2NO_2^+\cdot Cl^-$
$M_r$ = 402.73
Triclinic, $P\overline{1}$
$a$ = 9.263 (2) Å
$b$ = 10.432 (3) Å
$c$ = 11.490 (3) Å
$\alpha$ = 115.954 (3)°
$\beta$ = 93.925 (3)°
$\gamma$ = 103.015 (3)°
$V$ = 954.8 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.49 mm$^{-1}$
$T$ = 296 (2) K
0.60 × 0.38 × 0.18 mm

### Data collection

Bruker APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.782, $T_{max}$ = 0.915
8767 measured reflections
4422 independent reflections
3320 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.159
$S$ = 1.03
4422 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H2···Cl3 | 0.90 | 2.28 | 3.0890 (18) | 150 |
| N1—H1···Cl3$^{i}$ | 0.90 | 2.59 | 3.2447 (18) | 131 |

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2801).

## References

Bruker (2007). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Froimowitz, M., Wu, K.-M., George, C., VanDerveer, D., Shi, Q. & Deutsch, H. M. (1998). *Struct. Chem.* **9**, 295–303.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2008). E**64**, o2038 [doi:10.1107/S1600536808030742]

## (2*SR*,3*RS*)-Benzyl[4-chloro-1-(4-chlorophenyl)-1-methoxycarbonyl-2-butyl]-ammonium chloride

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### S1. Comment

The title molecule, (I), is a *β*-amino acid ester resulting from a rhodium-catalyzed C—H insertion reaction between methyl-(4-chlorophenyl)diazo acetate and Boc-protected *N*-benzyl-3-chloropropanamine. Full details will be published elsewhere.

### S2. Experimental

Colourless blocks of (I) were grown by diffusion of diethylether into 100 *μ*l of a solution containing about 5 mg of the title compound in methanol.

### S3. Refinement

The H atoms were positioned with idealized geometry (N–H = 0.90 Å, C–H = 0.93-0.98 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C, N) or 1.5$U_{eq}$(methyl C).

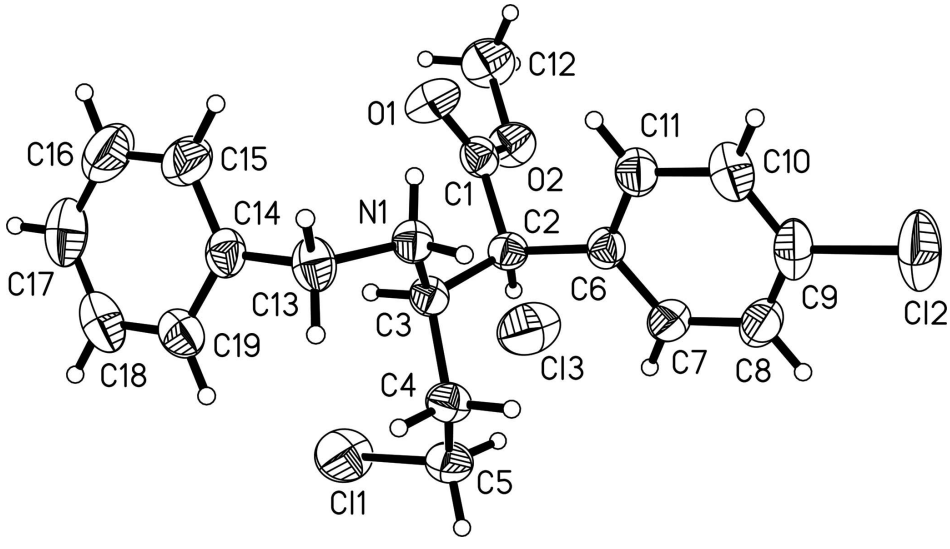


**Figure 1**

The molecular structure of (I). Displacement ellipsoids are shown at the 50% probability level and H-atoms are shown as spheres of arbitrary size.

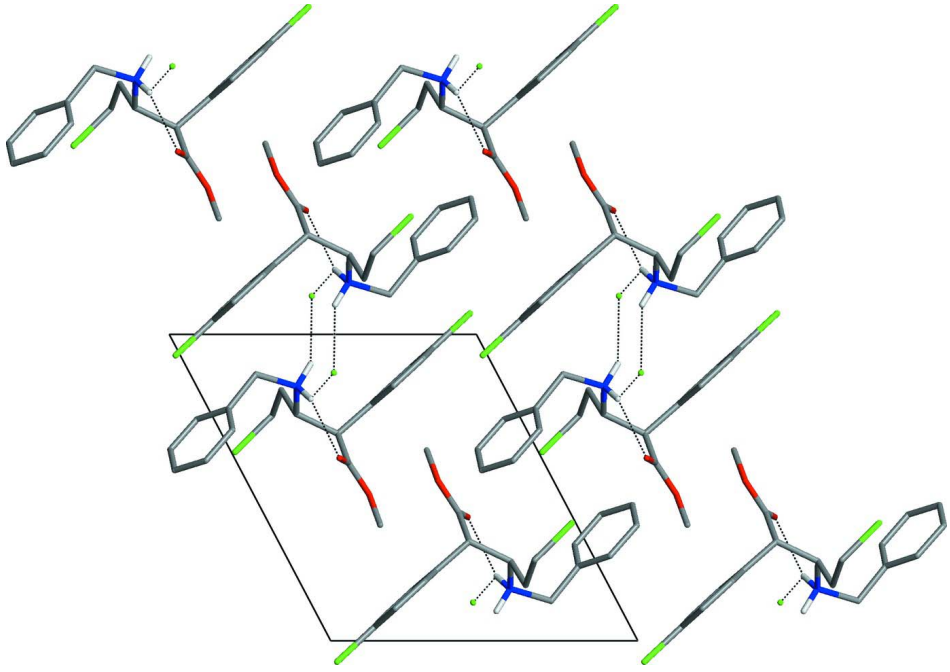

**Figure 2**

Molecular packing and unit cell of (I) viewed along the *a* axis. Hydrogen bonding is indicated by dashed lines, H-atoms bonded to C have been omitted for clarity.

**(2SR,3RS)-Benzyl[4-chloro-1-(4-chlorophenyl)-1-methoxycarbonyl- 2-butyl]ammonium chloride**

*Crystal data*

$C_{19}H_{22}Cl_2NO_2^+\cdot Cl^-$
$M_r = 402.73$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.263$ (2) Å
$b = 10.432$ (3) Å
$c = 11.490$ (3) Å
$\alpha = 115.954$ (3)°
$\beta = 93.925$ (3)°
$\gamma = 103.015$ (3)°
$V = 954.8$ (4) Å$^3$
$Z = 2$
$F(000) = 420$
$D_x = 1.401$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3509 reflections
$\theta = 2.0$–$28.7°$
$\mu = 0.49$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.60 × 0.38 × 0.18 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3 pixels mm$^{-1}$
sets of exposures each taken over 0.5° $\omega$ rotation scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.782$, $T_{max} = 0.915$
8767 measured reflections
4422 independent reflections
3320 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 28.7°$, $\theta_{min} = 2.0°$
$h = -12 \rightarrow 10$
$k = -13 \rightarrow 12$
$l = -15 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.159$
$S = 1.04$
4422 reflections
227 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
$w = 1/[\sigma^2(F_o^2) + (0.097P)^2 + 0.1562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.44$ e Å$^{-3}$
$\Delta\rho_{min} = -0.36$ e Å$^{-3}$

*Special details*

**Experimental**. Crystal grew over 48 h.

**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**. Data were collected by measuring three sets of exposures with the detector set at $2\theta = 29°$, crystal-to-detector distance 6.00 cm. Refinement of $F^2$ against ALL reflections.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.64470 (8) | 0.98821 (8) | 0.38456 (7) | 0.0691 (2) |
| Cl2 | 0.26825 (11) | −0.01534 (7) | −0.06864 (6) | 0.0787 (3) |
| Cl3 | 0.17315 (6) | 0.47020 (7) | −0.12520 (5) | 0.05352 (19) |
| O1 | 0.11480 (18) | 0.6582 (2) | 0.40412 (15) | 0.0512 (4) |
| O2 | 0.28993 (18) | 0.62358 (19) | 0.52192 (14) | 0.0473 (4) |
| N1 | 0.18786 (18) | 0.67376 (17) | 0.17013 (15) | 0.0330 (3) |
| H1 | 0.1142 | 0.6505 | 0.2107 | 0.040* |
| H2 | 0.1838 | 0.5903 | 0.0966 | 0.040* |
| C1 | 0.2347 (2) | 0.6371 (2) | 0.41927 (17) | 0.0346 (4) |
| C2 | 0.3435 (2) | 0.6218 (2) | 0.32432 (17) | 0.0321 (4) |
| H21 | 0.4452 | 0.6583 | 0.3773 | 0.039* |
| C3 | 0.3372 (2) | 0.7230 (2) | 0.25943 (17) | 0.0314 (4) |
| H31 | 0.3497 | 0.8237 | 0.3299 | 0.038* |
| C4 | 0.4634 (2) | 0.7305 (2) | 0.18192 (19) | 0.0377 (4) |
| H41 | 0.4571 | 0.6302 | 0.1166 | 0.045* |
| H42 | 0.4464 | 0.7852 | 0.1349 | 0.045* |
| C5 | 0.6210 (2) | 0.8022 (3) | 0.2633 (2) | 0.0457 (5) |
| H51 | 0.6930 | 0.8014 | 0.2058 | 0.055* |
| H52 | 0.6418 | 0.7446 | 0.3064 | 0.055* |
| C6 | 0.3211 (2) | 0.4594 (2) | 0.22692 (18) | 0.0338 (4) |
| C7 | 0.4464 (2) | 0.4091 (3) | 0.1945 (2) | 0.0431 (5) |
| H71 | 0.5425 | 0.4744 | 0.2344 | 0.052* |
| C8 | 0.4308 (3) | 0.2642 (3) | 0.1046 (2) | 0.0507 (6) |
| H81 | 0.5154 | 0.2315 | 0.0833 | 0.061* |
| C9 | 0.2888 (3) | 0.1685 (2) | 0.0466 (2) | 0.0495 (6) |
| C10 | 0.1623 (3) | 0.2137 (3) | 0.0776 (2) | 0.0494 (5) |

| | | | | |
|---|---|---|---|---|
| H101 | 0.0668 | 0.1469 | 0.0380 | 0.059* |
| C11 | 0.1778 (2) | 0.3591 (2) | 0.1681 (2) | 0.0423 (5) |
| H111 | 0.0925 | 0.3903 | 0.1899 | 0.051* |
| C12 | 0.1968 (3) | 0.6398 (3) | 0.6215 (2) | 0.0590 (7) |
| H121 | 0.2542 | 0.6480 | 0.6984 | 0.088* |
| H122 | 0.1100 | 0.5545 | 0.5872 | 0.088* |
| H123 | 0.1646 | 0.7278 | 0.6445 | 0.088* |
| C13 | 0.1553 (3) | 0.7857 (2) | 0.1302 (2) | 0.0416 (5) |
| H131 | 0.2240 | 0.7983 | 0.0735 | 0.050* |
| H132 | 0.0535 | 0.7461 | 0.0790 | 0.050* |
| C14 | 0.1697 (2) | 0.9353 (2) | 0.2434 (2) | 0.0387 (4) |
| C15 | 0.0533 (3) | 0.9580 (3) | 0.3120 (3) | 0.0589 (6) |
| H151 | −0.0319 | 0.8791 | 0.2907 | 0.071* |
| C16 | 0.0627 (4) | 1.0968 (3) | 0.4118 (3) | 0.0726 (8) |
| H161 | −0.0156 | 1.1104 | 0.4583 | 0.087* |
| C17 | 0.1861 (4) | 1.2151 (3) | 0.4434 (3) | 0.0646 (7) |
| H171 | 0.1906 | 1.3089 | 0.5097 | 0.077* |
| C18 | 0.3036 (3) | 1.1941 (3) | 0.3761 (2) | 0.0562 (6) |
| H181 | 0.3883 | 1.2736 | 0.3974 | 0.067* |
| C19 | 0.2947 (3) | 1.0547 (3) | 0.2771 (2) | 0.0456 (5) |
| H191 | 0.3742 | 1.0408 | 0.2322 | 0.055* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0507 (4) | 0.0516 (4) | 0.0684 (4) | −0.0046 (3) | 0.0023 (3) | 0.0063 (3) |
| Cl2 | 0.1402 (8) | 0.0425 (4) | 0.0514 (4) | 0.0395 (4) | 0.0239 (4) | 0.0128 (3) |
| Cl3 | 0.0418 (3) | 0.0546 (4) | 0.0430 (3) | 0.0064 (2) | 0.0086 (2) | 0.0077 (2) |
| O1 | 0.0410 (9) | 0.0740 (12) | 0.0479 (8) | 0.0263 (8) | 0.0165 (7) | 0.0306 (8) |
| O2 | 0.0516 (9) | 0.0586 (10) | 0.0389 (7) | 0.0191 (8) | 0.0122 (6) | 0.0269 (7) |
| N1 | 0.0316 (8) | 0.0309 (8) | 0.0339 (7) | 0.0081 (6) | 0.0027 (6) | 0.0138 (6) |
| C1 | 0.0379 (10) | 0.0281 (9) | 0.0313 (9) | 0.0053 (8) | 0.0045 (7) | 0.0103 (7) |
| C2 | 0.0278 (9) | 0.0334 (10) | 0.0332 (8) | 0.0074 (7) | 0.0039 (7) | 0.0149 (7) |
| C3 | 0.0289 (9) | 0.0284 (9) | 0.0306 (8) | 0.0048 (7) | 0.0015 (7) | 0.0106 (7) |
| C4 | 0.0349 (10) | 0.0377 (11) | 0.0375 (9) | 0.0058 (8) | 0.0077 (8) | 0.0170 (8) |
| C5 | 0.0351 (11) | 0.0457 (12) | 0.0527 (12) | 0.0067 (9) | 0.0097 (9) | 0.0220 (10) |
| C6 | 0.0390 (10) | 0.0330 (10) | 0.0340 (9) | 0.0136 (8) | 0.0097 (7) | 0.0176 (8) |
| C7 | 0.0411 (11) | 0.0451 (12) | 0.0520 (11) | 0.0188 (9) | 0.0169 (9) | 0.0261 (10) |
| C8 | 0.0627 (15) | 0.0514 (14) | 0.0564 (13) | 0.0329 (12) | 0.0298 (11) | 0.0307 (11) |
| C9 | 0.0855 (18) | 0.0354 (11) | 0.0353 (10) | 0.0277 (12) | 0.0167 (11) | 0.0175 (9) |
| C10 | 0.0565 (14) | 0.0359 (11) | 0.0491 (12) | 0.0099 (10) | −0.0034 (10) | 0.0175 (10) |
| C11 | 0.0390 (11) | 0.0360 (11) | 0.0491 (11) | 0.0110 (9) | 0.0030 (9) | 0.0180 (9) |
| C12 | 0.0731 (17) | 0.0678 (17) | 0.0396 (11) | 0.0207 (14) | 0.0212 (11) | 0.0263 (12) |
| C13 | 0.0464 (12) | 0.0381 (11) | 0.0405 (10) | 0.0126 (9) | −0.0013 (8) | 0.0194 (9) |
| C14 | 0.0373 (11) | 0.0360 (11) | 0.0447 (10) | 0.0133 (8) | 0.0010 (8) | 0.0201 (9) |
| C15 | 0.0377 (12) | 0.0492 (14) | 0.0818 (17) | 0.0139 (10) | 0.0119 (11) | 0.0227 (13) |
| C16 | 0.0671 (19) | 0.0614 (18) | 0.087 (2) | 0.0355 (15) | 0.0280 (16) | 0.0221 (15) |
| C17 | 0.083 (2) | 0.0421 (14) | 0.0609 (15) | 0.0286 (14) | 0.0017 (14) | 0.0136 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18 | 0.0662 (16) | 0.0382 (12) | 0.0588 (14) | 0.0058 (11) | −0.0061 (12) | 0.0246 (11) |
| C19 | 0.0476 (12) | 0.0427 (12) | 0.0502 (11) | 0.0100 (9) | 0.0065 (9) | 0.0267 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C5 | 1.776 (2) | C8—C9 | 1.370 (4) |
| Cl2—C9 | 1.745 (2) | C8—H81 | 0.9300 |
| O1—C1 | 1.196 (3) | C9—C10 | 1.372 (3) |
| O2—C1 | 1.330 (2) | C10—C11 | 1.379 (3) |
| O2—C12 | 1.454 (3) | C10—H101 | 0.9300 |
| N1—C3 | 1.502 (2) | C11—H111 | 0.9300 |
| N1—C13 | 1.508 (3) | C12—H121 | 0.9600 |
| N1—H1 | 0.9000 | C12—H122 | 0.9600 |
| N1—H2 | 0.9000 | C12—H123 | 0.9600 |
| C1—C2 | 1.517 (3) | C13—C14 | 1.501 (3) |
| C2—C6 | 1.522 (3) | C13—H131 | 0.9700 |
| C2—C3 | 1.544 (3) | C13—H132 | 0.9700 |
| C2—H21 | 0.9800 | C14—C15 | 1.381 (3) |
| C3—C4 | 1.526 (3) | C14—C19 | 1.381 (3) |
| C3—H31 | 0.9800 | C15—C16 | 1.376 (4) |
| C4—C5 | 1.508 (3) | C15—H151 | 0.9300 |
| C4—H41 | 0.9700 | C16—C17 | 1.370 (4) |
| C4—H42 | 0.9700 | C16—H161 | 0.9300 |
| C5—H51 | 0.9700 | C17—C18 | 1.380 (4) |
| C5—H52 | 0.9700 | C17—H171 | 0.9300 |
| C6—C7 | 1.387 (3) | C18—C19 | 1.379 (3) |
| C6—C11 | 1.395 (3) | C18—H181 | 0.9300 |
| C7—C8 | 1.374 (3) | C19—H191 | 0.9300 |
| C7—H71 | 0.9300 | | |

| | | | |
|---|---|---|---|
| C1—O2—C12 | 116.08 (18) | C9—C8—H81 | 120.4 |
| C3—N1—C13 | 115.50 (15) | C7—C8—H81 | 120.4 |
| C3—N1—H1 | 108.4 | C8—C9—C10 | 121.5 (2) |
| C13—N1—H1 | 108.4 | C8—C9—Cl2 | 119.32 (19) |
| C3—N1—H2 | 108.4 | C10—C9—Cl2 | 119.2 (2) |
| C13—N1—H2 | 108.4 | C9—C10—C11 | 119.5 (2) |
| H1—N1—H2 | 107.5 | C9—C10—H101 | 120.3 |
| O1—C1—O2 | 124.21 (18) | C11—C10—H101 | 120.3 |
| O1—C1—C2 | 124.68 (17) | C10—C11—C6 | 120.2 (2) |
| O2—C1—C2 | 111.11 (17) | C10—C11—H111 | 119.9 |
| C1—C2—C6 | 111.18 (15) | C6—C11—H111 | 119.9 |
| C1—C2—C3 | 111.11 (15) | O2—C12—H121 | 109.5 |
| C6—C2—C3 | 114.25 (14) | O2—C12—H122 | 109.5 |
| C1—C2—H21 | 106.6 | H121—C12—H122 | 109.5 |
| C6—C2—H21 | 106.6 | O2—C12—H123 | 109.5 |
| C3—C2—H21 | 106.6 | H121—C12—H123 | 109.5 |
| N1—C3—C4 | 109.14 (15) | H122—C12—H123 | 109.5 |
| N1—C3—C2 | 111.71 (14) | C14—C13—N1 | 114.43 (16) |

| | | | |
|---|---|---|---|
| C4—C3—C2 | 112.34 (16) | C14—C13—H131 | 108.7 |
| N1—C3—H31 | 107.8 | N1—C13—H131 | 108.7 |
| C4—C3—H31 | 107.8 | C14—C13—H132 | 108.7 |
| C2—C3—H31 | 107.8 | N1—C13—H132 | 108.7 |
| C5—C4—C3 | 115.28 (16) | H131—C13—H132 | 107.6 |
| C5—C4—H41 | 108.5 | C15—C14—C19 | 118.5 (2) |
| C3—C4—H41 | 108.5 | C15—C14—C13 | 120.1 (2) |
| C5—C4—H42 | 108.5 | C19—C14—C13 | 121.3 (2) |
| C3—C4—H42 | 108.5 | C16—C15—C14 | 120.4 (2) |
| H41—C4—H42 | 107.5 | C16—C15—H151 | 119.8 |
| C4—C5—Cl1 | 111.82 (16) | C14—C15—H151 | 119.8 |
| C4—C5—H51 | 109.3 | C17—C16—C15 | 120.8 (3) |
| Cl1—C5—H51 | 109.3 | C17—C16—H161 | 119.6 |
| C4—C5—H52 | 109.3 | C15—C16—H161 | 119.6 |
| Cl1—C5—H52 | 109.3 | C16—C17—C18 | 119.6 (2) |
| H51—C5—H52 | 107.9 | C16—C17—H171 | 120.2 |
| C7—C6—C11 | 118.70 (19) | C18—C17—H171 | 120.2 |
| C7—C6—C2 | 119.31 (18) | C19—C18—C17 | 119.6 (2) |
| C11—C6—C2 | 121.99 (17) | C19—C18—H181 | 120.2 |
| C8—C7—C6 | 121.0 (2) | C17—C18—H181 | 120.2 |
| C8—C7—H71 | 119.5 | C18—C19—C14 | 121.2 (2) |
| C6—C7—H71 | 119.5 | C18—C19—H191 | 119.4 |
| C9—C8—C7 | 119.1 (2) | C14—C19—H191 | 119.4 |

| | | | |
|---|---|---|---|
| C1—C2—C3—C4 | 170.19 (15) | C3—C2—C6—C11 | −84.9 (2) |
| C2—C3—C4—C5 | −65.1 (2) | C11—C6—C7—C8 | 1.2 (3) |
| C3—C4—C5—Cl1 | −59.2 (2) | C2—C6—C7—C8 | −178.37 (18) |
| C3—C2—C1—O2 | −145.64 (16) | C6—C7—C8—C9 | −0.2 (3) |
| C2—C1—O2—C12 | 178.60 (18) | C7—C8—C9—C10 | −0.8 (3) |
| C1—C2—C6—C7 | −138.62 (18) | C7—C8—C9—Cl2 | 179.55 (17) |
| C2—C3—N1—C13 | 164.81 (16) | C8—C9—C10—C11 | 0.7 (3) |
| C3—N1—C13—C14 | −53.8 (2) | Cl2—C9—C10—C11 | −179.63 (16) |
| N1—C13—C14—C15 | −80.7 (3) | C9—C10—C11—C6 | 0.3 (3) |
| C12—O2—C1—O1 | −1.5 (3) | C7—C6—C11—C10 | −1.3 (3) |
| O1—C1—C2—C6 | −93.9 (2) | C2—C6—C11—C10 | 178.28 (18) |
| O2—C1—C2—C6 | 85.91 (19) | N1—C13—C14—C19 | 102.7 (2) |
| O1—C1—C2—C3 | 34.5 (3) | C19—C14—C15—C16 | −0.1 (4) |
| C13—N1—C3—C4 | −70.3 (2) | C13—C14—C15—C16 | −176.8 (2) |
| C1—C2—C3—N1 | −66.78 (18) | C14—C15—C16—C17 | 1.1 (5) |
| C6—C2—C3—N1 | 60.0 (2) | C15—C16—C17—C18 | −1.4 (5) |
| C6—C2—C3—C4 | −63.0 (2) | C16—C17—C18—C19 | 0.7 (4) |
| N1—C3—C4—C5 | 170.40 (17) | C17—C18—C19—C14 | 0.3 (3) |
| C3—C2—C6—C7 | 94.6 (2) | C15—C14—C19—C18 | −0.6 (3) |
| C1—C2—C6—C11 | 41.8 (2) | C13—C14—C19—C18 | 176.10 (19) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H2···Cl3 | 0.90 | 2.28 | 3.0890 (18) | 150 |
| N1—H1···Cl3$^{i}$ | 0.90 | 2.59 | 3.2447 (18) | 131 |

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