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# 2-(4-Fluorophenyl)-1-(4-pyridyl)cyclopentan-1-ol

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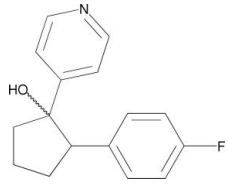
Key indicators: single-crystal X-ray study; $T$ = 193 K; mean $\sigma$(C–C) = 0.010 Å; $R$ factor = 0.125; $wR$ factor = 0.361; data-to-parameter ratio = 14.6.

The crystal structure of the title compound, $C_{16}H_{16}FNO$, was determined as part of a study of the biological activity of pyridine-substituted cyclopentene derivatives as p38 mitogen-activated protein kinase (MAPK) inhibitors. The 4-fluorophenyl and 4-pyridyl rings are *trans* positioned with respect to each other. The compound exists as a racemic mixture. The synthesis was achieved *via* direct interaction between the reactive complex Grignard reagent PyMgCl·LiCl and the enolizable ketone 4-fluorophenylcyclopentanone with the assistance of the neodymium salt catalyst $NdCl_3$·2LiCl. The crystal packing is characterized by zigzag chains of molecules, which are connected by O—H···N hydrogen bonds running along the *b* axis.

## Related literature

In the title compound, the vicinal substituents are in a *trans* position with respect to each other; this is different from the structure of other related five-membered rings, as exemplified by the pyridinylimidazole SB203580 inhibitor for p38 MAPK (Wang *et al.*, 1998; Laufer *et al.*, 2006). For further literature, see Abu Thaher *et al.* (2007) and references therein.

For related literature, see: Kaminska (2005); Krasovskiy & Knochel (2004); Krasovskiy *et al.* (2006); Wagner & Laufer (2006).




## Experimental

### Crystal data

$C_{16}H_{16}FNO$
$M_r$ = 257.30
Monoclinic, $P2_1/c$
$a$ = 11.7228 (8) Å
$b$ = 13.6606 (8) Å
$c$ = 8.6194 (11) Å
$\beta$ = 104.366 (10)°
$V$ = 1337.2 (2) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 0.73 mm$^{-1}$
$T$ = 193 (2) K
0.30 × 0.30 × 0.06 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
2701 measured reflections
2523 independent reflections
1235 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.050
3 standard reflections
frequency: 60 min
intensity decay: 5%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.126
$wR(F^2)$ = 0.361
$S$ = 1.28
2523 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.67 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O6—H6···N10$^{i}$ | 0.84 | 1.95 | 2.758 (7) | 161 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CORINC* (Dräger & Gattow, 1971); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2433).

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# supplementary materials

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# 2-(4-Fluorophenyl)-1-(4-pyridyl)cyclopentan-1-ol

**B. Abu Thaher, D. Schollmeyer and S. Laufer**

## Comment

Compound **4** was prepared in the course of our study on cyclopentene derivatives bearing the typical vicinal 4-pyridyl and 4-fluorophenyl pharmacophores of MAP Kinase inhibitors. Pyridinylimidazoles are described in the literature as inhibitors for p38 MAP Kinase (Wagner *et al.*, 2006; Kaminska, 2005). The prototypical pyridinylimidazole SB 203580 is one of the best studied p38 inhibitors reported until now. Figure 1 shows the most important interactions between the ATP binding sites of p38 kinase and the imidazole inhibitor SB203580 (Wang *et al.*, 1998; Laufer *et al.*, 2006). The 4-fluorophenyl ring of SB203580 occupies a hydrophobic back pocket gaining selectivity. Vicinal to this interaction site, 4-pyridinyl moiety forms a hydrogen bond from the backbone NH group of Met 109 of p38 MAP Kinase (Fig. 1).

Meanwhile, the importance of a further hydrogen bond between N3 of the imidazole core and Lys53 of p38 MAP Kinase, as shown in figure 1, is not yet clear and the speculation about its significance is not settled. Based on this concept, replacement of imidazole core by a cyclopentene ring would require the preparation of 2-fluorophenyl-1-pyridinyl cyclopentanol **4** as a key compound for such comparative bioassay study. Going from the data obtained from the X-ray structure of compound **4** (Figs. 2 and 3), it is impossible for the vicinal 4-fluorophenyl and 4-pyridinyl groups (due to their location in *trans* position to each other) to exert their expected functions with p38 MAPK as described above in case of SB203580 inhibitor (Fig. 1).

So, the loss of the biological activity of compound **4** can not be attributed just to the absence of the nitrogen atoms in the cyclopentane core itself. Accordingly, and based on this result, we plan to prepare cyclopentene derivatives which have vicinal 4-fluorophenyl and 4-pyridinyl groups in *cis* orientation in order to get more accurate and comparable information about the extent of the importance of the hydrogen bond between N3 of the imidazole core and Lys 53 of P38 MAP Kinase in terms of its biological activity.

## Experimental

Compound **4** was obtained by reacting 1.0 mmol of 2-(4-fluorophenyl)-1-cyclopentanone **3** to 1.05 mmol N dC $l_3$·2LiCl (Krasovskiy *et al.*, 2006) under dry conditions, followed by adding the prepared complex Grignard PyMgCl·LiCl, from *i*PrMgCl·LiCl by exchange reaction (Krasovskiy and Knochel, 2004), to the first reaction at 273 K and then at rt for 8–10 h. When the reaction was completed, saturated aqueous $NH_4Cl$ (2 ml) and water (10 ml) were added. The aqueous layer was extracted with diethyl ether (4 *x* 10 ml), and the combined organic extracts were dried ($Na_2SO_4$) and evaporated to dryness. The crude product was purified by flash column chromatography (n-hexane / ethyl acetate, 3:1, *v*/*v*) giving **4** (yield 58.5°) as colorless, crystalline needles. For X-ray analysis suitable crystals of compund 4 were obtained by slow evaporation at 298 K of methanol - chloroform (2:1) solution.

### Refinement

Hydrogen atoms attached to carbons were placed at calculated positions with C—H=0.95A% (aromatic) or 0.99–1.00 Å ($sp^3$ C-atom). Hydrogen atom attached to O6 was located in a difference Fourier map. The isotropic displacement parameters were set to 1.2–1.5 times of the $U_{eq}$ of the parent atom.

### Figures

Fig. 1. Schematic drawing of important interactions between the prototypical pyridin-4-yl imidazole inhibitor SB 203580 and the ATP binding site of p38.

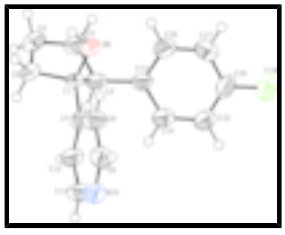

Fig. 2. The molecular structure of 4. Dislacement ellipsoids are drawn at the 50% probability level and H atoms are depicted as circles of arbitrary radius.

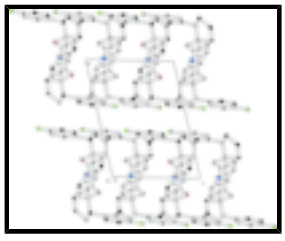

Fig. 3. Part of the packing of 4, viewed along the *b* axis showing the racemic modification of the molecule. H atoms are omitted. The packing is influenced by O—H···N hydrogen bonds along the *b* axis.

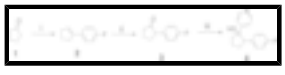

Fig. 4. Chemical preparation of 4. Reagents and conditions: (i) 4-fluorophenylmagnesium-bromide, ether, reflux; (ii) $H_2O_2$, formic acid; (iii) $NdCl_3$·2LiCl, 1 h and then 2 equivalents PyMgCl·LiCl, 273 K, 8–10 h.

### 2-(4-Fluorophenyl)-1-(4-pyridyl)cyclopentan-1-ol

*Crystal data*

| | |
|---|---|
| $C_{16}H_{16}FNO$ | $F_{000}$ = 544 |
| $M_r$ = 257.30 | $D_x$ = 1.278 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation<br>λ = 1.54178 Å |
| Hall symbol: -P 2ybc | Cell parameters from 25 reflections |
| $a$ = 11.7228 (8) Å | θ = 20–25.7º |
| $b$ = 13.6606 (8) Å | μ = 0.73 mm$^{-1}$ |
| $c$ = 8.6194 (11) Å | $T$ = 193 (2) K |
| β = 104.366 (10)º | Plate, colourless |
| $V$ = 1337.2 (2) Å$^3$ | 0.30 × 0.30 × 0.06 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | $\theta_{max}$ = 70.3º |
| Monochromator: graphite | $\theta_{min}$ = 3.9º |
| $T$ = 193(2) K | $h$ = −14→13 |
| ω/2θ scans | $k$ = 0→16 |
| Absorption correction: none | $l$ = 0→10 |
| 2701 measured reflections | 3 standard reflections |
| 2523 independent reflections | every 60 min |
| 1235 reflections with $I > 2\sigma(I)$ | intensity decay: 5% |
| $R_{int}$ = 0.050 | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.126 | $[1 + -\exp(-4.00(\sin\theta/\lambda)^2)]/[\sigma^2(F_o^2) + (0.08P)^2 + \sin\theta/\lambda]$, where $P = 0.33333F_o^2 + 0.66667F_c^2$ |
| $wR(F^2)$ = 0.361 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 1.28 | $\Delta\rho_{max}$ = 0.69 e Å$^{-3}$ |
| 2523 reflections | $\Delta\rho_{min}$ = −0.67 e Å$^{-3}$ |
| 173 parameters | Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.006 (4) |
| Secondary atom site location: difference Fourier map | |

*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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1840 (6) | 0.4649 (4) | 0.8347 (8) | 0.0455 (17) |
| C2 | 0.3152 (6) | 0.4837 (4) | 0.8462 (8) | 0.0469 (17) |

| | | | | |
|---|---|---|---|---|
| H2 | 0.3433 | 0.5334 | 0.9323 | 0.056* |
| C3 | 0.3736 (7) | 0.3850 (5) | 0.9078 (10) | 0.060 (2) |
| H3A | 0.3741 | 0.3405 | 0.8173 | 0.072* |
| H3B | 0.4556 | 0.3951 | 0.9709 | 0.072* |
| C4 | 0.2981 (8) | 0.3433 (5) | 1.0124 (11) | 0.064 (2) |
| H4A | 0.3429 | 0.3428 | 1.1260 | 0.077* |
| H4B | 0.2747 | 0.2752 | 0.9798 | 0.077* |
| C5 | 0.1886 (7) | 0.4085 (4) | 0.9909 (9) | 0.0553 (19) |
| H5A | 0.1966 | 0.4540 | 1.0824 | 0.066* |
| H5B | 0.1168 | 0.3684 | 0.9812 | 0.066* |
| O6 | 0.1394 (4) | 0.4049 (3) | 0.6997 (5) | 0.0528 (13) |
| H6 | 0.1084 | 0.3547 | 0.7282 | 0.079* |
| C7 | 0.1137 (6) | 0.5605 (4) | 0.8200 (9) | 0.0463 (17) |
| C8 | 0.0127 (6) | 0.5733 (5) | 0.6989 (10) | 0.0525 (18) |
| H8 | −0.0170 | 0.5217 | 0.6263 | 0.063* |
| C9 | −0.0443 (8) | 0.6628 (5) | 0.6854 (10) | 0.061 (2) |
| H9 | −0.1124 | 0.6709 | 0.5997 | 0.074* |
| N10 | −0.0107 (6) | 0.7380 (4) | 0.7833 (9) | 0.0617 (18) |
| C11 | 0.0856 (7) | 0.7239 (5) | 0.9014 (11) | 0.061 (2) |
| H11 | 0.1128 | 0.7764 | 0.9734 | 0.073* |
| C12 | 0.1476 (7) | 0.6374 (4) | 0.9246 (10) | 0.0550 (19) |
| H12 | 0.2141 | 0.6308 | 1.0131 | 0.066* |
| C13 | 0.3400 (6) | 0.5238 (4) | 0.6929 (9) | 0.0465 (16) |
| C14 | 0.3684 (7) | 0.6227 (5) | 0.6829 (10) | 0.0548 (19) |
| H14 | 0.3739 | 0.6635 | 0.7737 | 0.066* |
| C15 | 0.3884 (7) | 0.6625 (5) | 0.5464 (10) | 0.061 (2) |
| H15 | 0.4086 | 0.7297 | 0.5425 | 0.073* |
| C16 | 0.3788 (7) | 0.6039 (5) | 0.4171 (10) | 0.063 (2) |
| C17 | 0.3516 (7) | 0.5067 (5) | 0.4207 (10) | 0.061 (2) |
| H17 | 0.3454 | 0.4670 | 0.3285 | 0.074* |
| C18 | 0.3332 (6) | 0.4667 (5) | 0.5597 (9) | 0.0558 (19) |
| H18 | 0.3157 | 0.3990 | 0.5632 | 0.067* |
| F19 | 0.3971 (5) | 0.6414 (3) | 0.2785 (6) | 0.0785 (16) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.073 (4) | 0.021 (2) | 0.050 (4) | −0.004 (2) | 0.030 (4) | −0.008 (2) |
| C2 | 0.057 (4) | 0.028 (2) | 0.058 (4) | 0.002 (2) | 0.018 (3) | −0.007 (3) |
| C3 | 0.066 (5) | 0.038 (3) | 0.077 (5) | 0.009 (3) | 0.021 (4) | 0.003 (3) |
| C4 | 0.088 (6) | 0.036 (3) | 0.069 (5) | 0.006 (3) | 0.023 (4) | 0.011 (3) |
| C5 | 0.084 (5) | 0.030 (3) | 0.059 (4) | −0.006 (3) | 0.031 (4) | 0.003 (3) |
| O6 | 0.082 (3) | 0.0270 (18) | 0.056 (3) | −0.010 (2) | 0.030 (3) | −0.0010 (18) |
| C7 | 0.047 (4) | 0.033 (3) | 0.067 (5) | 0.000 (2) | 0.030 (4) | 0.001 (3) |
| C8 | 0.048 (4) | 0.043 (3) | 0.071 (5) | 0.001 (3) | 0.022 (4) | −0.006 (3) |
| C9 | 0.074 (5) | 0.054 (4) | 0.063 (5) | 0.012 (3) | 0.030 (4) | 0.003 (4) |
| N10 | 0.071 (5) | 0.045 (3) | 0.077 (5) | 0.014 (3) | 0.036 (4) | 0.005 (3) |
| C11 | 0.061 (5) | 0.041 (3) | 0.086 (6) | 0.009 (3) | 0.028 (5) | −0.013 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.068 (5) | 0.035 (3) | 0.069 (5) | 0.005 (3) | 0.029 (4) | 0.000 (3) |
| C13 | 0.051 (4) | 0.030 (3) | 0.065 (4) | 0.004 (2) | 0.026 (3) | −0.002 (3) |
| C14 | 0.066 (5) | 0.039 (3) | 0.065 (5) | 0.003 (3) | 0.026 (4) | −0.001 (3) |
| C15 | 0.079 (5) | 0.038 (3) | 0.076 (6) | 0.004 (3) | 0.036 (4) | 0.007 (3) |
| C16 | 0.075 (5) | 0.048 (4) | 0.077 (6) | 0.010 (3) | 0.040 (5) | 0.023 (4) |
| C17 | 0.072 (5) | 0.056 (4) | 0.061 (5) | 0.004 (3) | 0.026 (4) | −0.012 (4) |
| C18 | 0.065 (5) | 0.037 (3) | 0.073 (5) | −0.006 (3) | 0.029 (4) | −0.002 (3) |
| F19 | 0.111 (4) | 0.066 (3) | 0.070 (3) | 0.008 (2) | 0.044 (3) | 0.022 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—O6 | 1.413 (7) | C8—H8 | 0.9500 |
| C1—C7 | 1.533 (8) | C9—N10 | 1.326 (10) |
| C1—C2 | 1.538 (9) | C9—H9 | 0.9500 |
| C1—C5 | 1.541 (9) | N10—C11 | 1.333 (11) |
| C2—C13 | 1.523 (9) | C11—C12 | 1.375 (9) |
| C2—C3 | 1.545 (9) | C11—H11 | 0.9500 |
| C2—H2 | 1.0000 | C12—H12 | 0.9500 |
| C3—C4 | 1.522 (10) | C13—C18 | 1.374 (9) |
| C3—H3A | 0.9900 | C13—C14 | 1.400 (9) |
| C3—H3B | 0.9900 | C14—C15 | 1.368 (10) |
| C4—C5 | 1.536 (11) | C14—H14 | 0.9500 |
| C4—H4A | 0.9900 | C15—C16 | 1.354 (11) |
| C4—H4B | 0.9900 | C15—H15 | 0.9500 |
| C5—H5A | 0.9900 | C16—F19 | 1.365 (8) |
| C5—H5B | 0.9900 | C16—C17 | 1.368 (10) |
| O6—H6 | 0.8400 | C17—C18 | 1.381 (10) |
| C7—C12 | 1.377 (9) | C17—H17 | 0.9500 |
| C7—C8 | 1.382 (10) | C18—H18 | 0.9500 |
| C8—C9 | 1.384 (10) | | |
| O6—C1—C7 | 110.2 (6) | C8—C7—C1 | 120.8 (6) |
| O6—C1—C2 | 108.0 (5) | C7—C8—C9 | 118.7 (7) |
| C7—C1—C2 | 111.8 (4) | C7—C8—H8 | 120.6 |
| O6—C1—C5 | 110.8 (4) | C9—C8—H8 | 120.6 |
| C7—C1—C5 | 113.6 (5) | N10—C9—C8 | 124.7 (9) |
| C2—C1—C5 | 102.1 (6) | N10—C9—H9 | 117.6 |
| C13—C2—C1 | 114.0 (6) | C8—C9—H9 | 117.6 |
| C13—C2—C3 | 116.6 (5) | C9—N10—C11 | 115.8 (6) |
| C1—C2—C3 | 103.1 (5) | N10—C11—C12 | 123.5 (7) |
| C13—C2—H2 | 107.5 | N10—C11—H11 | 118.2 |
| C1—C2—H2 | 107.5 | C12—C11—H11 | 118.2 |
| C3—C2—H2 | 107.5 | C11—C12—C7 | 120.2 (8) |
| C4—C3—C2 | 104.9 (6) | C11—C12—H12 | 119.9 |
| C4—C3—H3A | 110.8 | C7—C12—H12 | 119.9 |
| C2—C3—H3A | 110.8 | C18—C13—C14 | 117.5 (6) |
| C4—C3—H3B | 110.8 | C18—C13—C2 | 122.5 (5) |
| C2—C3—H3B | 110.8 | C14—C13—C2 | 120.0 (6) |
| H3A—C3—H3B | 108.8 | C15—C14—C13 | 122.1 (7) |
| C3—C4—C5 | 107.6 (6) | C15—C14—H14 | 119.0 |

| | | | |
|---|---|---|---|
| C3—C4—H4A | 110.2 | C13—C14—H14 | 119.0 |
| C5—C4—H4A | 110.2 | C16—C15—C14 | 118.4 (6) |
| C3—C4—H4B | 110.2 | C16—C15—H15 | 120.8 |
| C5—C4—H4B | 110.2 | C14—C15—H15 | 120.8 |
| H4A—C4—H4B | 108.5 | C15—C16—F19 | 120.0 (6) |
| C4—C5—C1 | 104.0 (5) | C15—C16—C17 | 121.8 (7) |
| C4—C5—H5A | 110.9 | F19—C16—C17 | 118.2 (7) |
| C1—C5—H5A | 110.9 | C16—C17—C18 | 119.4 (7) |
| C4—C5—H5B | 110.9 | C16—C17—H17 | 120.3 |
| C1—C5—H5B | 110.9 | C18—C17—H17 | 120.3 |
| H5A—C5—H5B | 109.0 | C13—C18—C17 | 120.8 (6) |
| C1—O6—H6 | 109.3 | C13—C18—H18 | 119.6 |
| C12—C7—C8 | 116.9 (6) | C17—C18—H18 | 119.6 |
| C12—C7—C1 | 122.3 (7) | | |
| O6—C1—C2—C13 | 53.2 (6) | C7—C8—C9—N10 | −1.7 (11) |
| C7—C1—C2—C13 | −68.2 (7) | C8—C9—N10—C11 | 0.4 (11) |
| C5—C1—C2—C13 | 170.0 (5) | C9—N10—C11—C12 | −0.6 (11) |
| O6—C1—C2—C3 | −74.2 (6) | N10—C11—C12—C7 | 2.2 (11) |
| C7—C1—C2—C3 | 164.4 (6) | C8—C7—C12—C11 | −3.3 (9) |
| C5—C1—C2—C3 | 42.6 (6) | C1—C7—C12—C11 | 176.3 (6) |
| C13—C2—C3—C4 | −157.3 (6) | C1—C2—C13—C18 | −73.7 (7) |
| C1—C2—C3—C4 | −31.6 (7) | C3—C2—C13—C18 | 46.4 (9) |
| C2—C3—C4—C5 | 8.3 (9) | C1—C2—C13—C14 | 104.9 (7) |
| C3—C4—C5—C1 | 18.1 (8) | C3—C2—C13—C14 | −135.0 (7) |
| O6—C1—C5—C4 | 77.5 (7) | C18—C13—C14—C15 | 0.3 (11) |
| C7—C1—C5—C4 | −157.8 (6) | C2—C13—C14—C15 | −178.3 (7) |
| C2—C1—C5—C4 | −37.3 (6) | C13—C14—C15—C16 | 0.8 (12) |
| O6—C1—C7—C12 | −171.5 (5) | C14—C15—C16—F19 | 179.4 (7) |
| C2—C1—C7—C12 | −51.4 (8) | C14—C15—C16—C17 | −1.0 (12) |
| C5—C1—C7—C12 | 63.5 (8) | C15—C16—C17—C18 | 0.0 (12) |
| O6—C1—C7—C8 | 8.0 (7) | F19—C16—C17—C18 | 179.7 (7) |
| C2—C1—C7—C8 | 128.2 (6) | C14—C13—C18—C17 | −1.3 (11) |
| C5—C1—C7—C8 | −116.9 (7) | C2—C13—C18—C17 | 177.3 (7) |
| C12—C7—C8—C9 | 3.0 (9) | C16—C17—C18—C13 | 1.1 (11) |
| C1—C7—C8—C9 | −176.6 (6) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O6—H6···N10$^{i}$ | 0.84 | 1.95 | 2.758 (7) | 161 |

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

**Fig. 1**

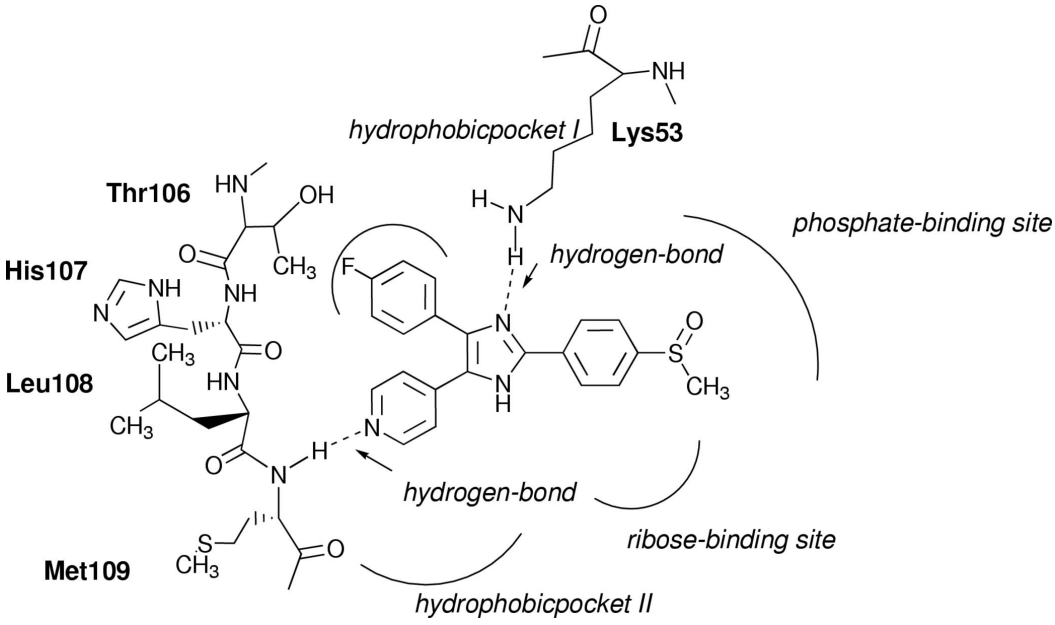
hydrophobicpocket I
Lys53
Thr106
His107
Leu108
Met109
phosphate-binding site
hydrogen-bond
hydrogen-bond
ribose-binding site
hydrophobicpocket II

**Fig. 2**

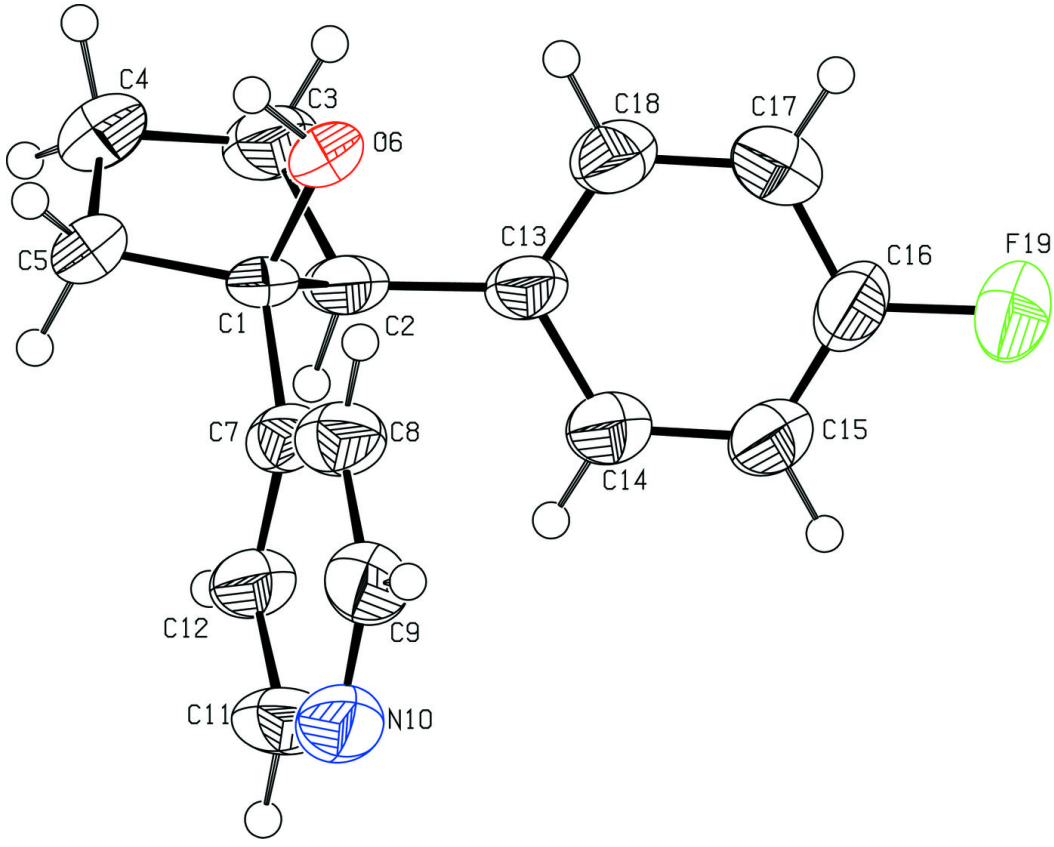

**Fig. 3**

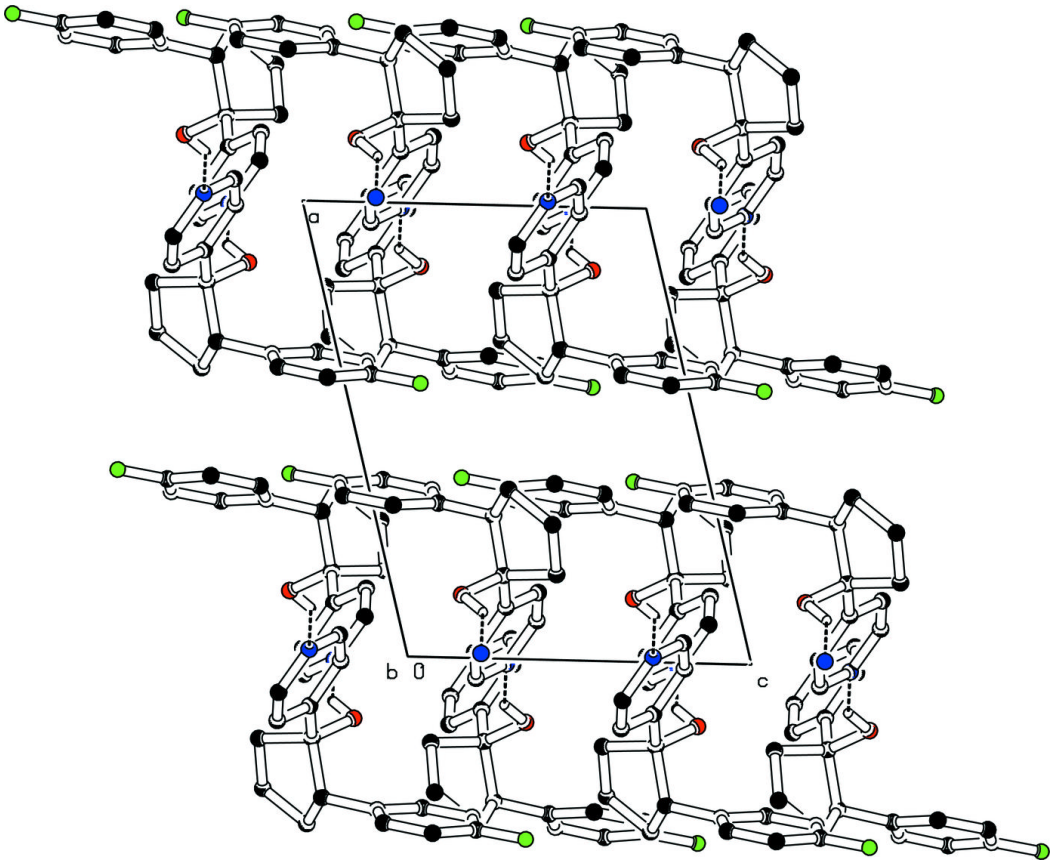

**Fig. 4**