



Crystal structure of luliconazole

Anna Ben^{a,b,*} and Lilianna Chęcińska^b

^aUniversity of Lodz Doctoral School of Exact and Natural Sciences, Narutowicza 68, 90-136 Łódź, Poland, and ^bUniversity of Lodz, Faculty of Chemistry, Pomorska 163/165, 90-236 Łódź, Poland. *Correspondence e-mail: anna.ben@edu.uni.lodz.pl

Received 20 November 2024

Accepted 4 December 2024

Edited by L. Van Meervelt, Katholieke Universiteit Leuven, Belgium

Keywords: luliconazole; crystal structure; Hirshfeld surface analysis.

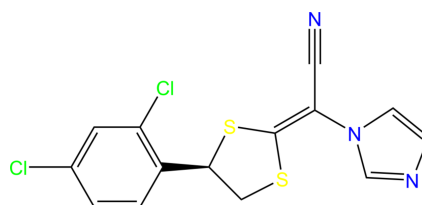
CCDC reference: 2407813

Supporting information: this article has supporting information at journals.iucr.org/e

The crystal structure of luliconazole {LCZ; C₁₄H₉Cl₂N₃S₂; systematic name: (*E*)-[(4*R*)-4-(2,4-dichlorophenyl)-1,3-dithiolan-2-ylidene](1*H*-imidazol-1-yl)acetonitrile} is reported. In the molecule of the title compound, the dithiolane ring adopts an envelope conformation, while the dichlorophenyl ring exhibits disorder. In the crystal packing of luliconazole, only two intermolecular C–H...N hydrogen bonds are observed. Hirshfeld surface analysis reveals that the most dominant contacts are H...N/N...H, H...Cl/Cl...H, H...H and C...H/H...C.

1. Chemical context

Luliconazole {LCZ; C₁₄H₉Cl₂N₃S₂; CAS No. 187164-19-8; systematic name: (*E*)-[(4*R*)-4-(2,4-dichlorophenyl)-1,3-dithiolan-2-ylidene](1*H*-imidazol-1-yl)acetonitrile} is a prominent antifungal agent and belongs to theazole class of drugs, specifically imidazole derivatives. The compound possesses a distinctive chemical structure, enhanced by the incorporation of an imidazole moiety into the ketene dithioacetate framework. This structural modification retains the broad antifungal spectrum of imidazole drugs, while achieving high potency against filamentous fungi, including dermatophytes (Koga *et al.*, 2012).

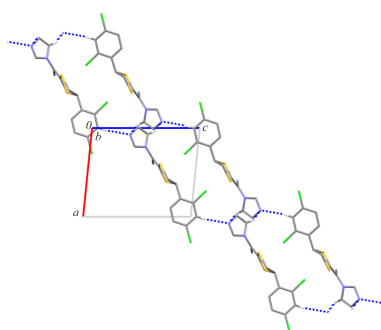


Luliconazole, as the *R*-enantiomer, exhibits significantly greater antifungal activity compared to lanoconazole, which exists as a racemic mixture (Deepshikha & Subhash, 2014). The key distinction between these two compounds lies in their stereochemistry: lanoconazole is a racemic compound, while luliconazole is the pure *R*-enantiomer. Interestingly, the *S*-enantiomers of both compounds are inactive as antifungal agents, making LCZ inherently more potent (Niwano *et al.*, 1998).

This article provides a detailed structural analysis of the pure drug luliconazole, which has not previously been reported in the literature.

2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1. It crystallizes in the monoclinic crystal system, space



OPEN ACCESS

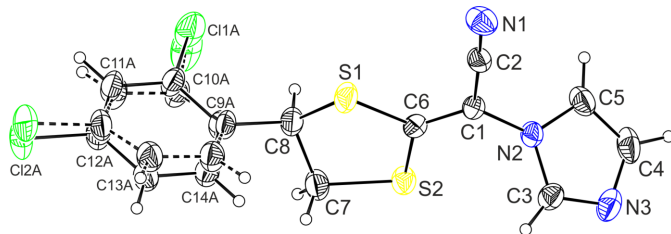
Published under a CC BY 4.0 licence

Table 1Dihedral angles ($^{\circ}$) between the best planes in LCZ-structures.

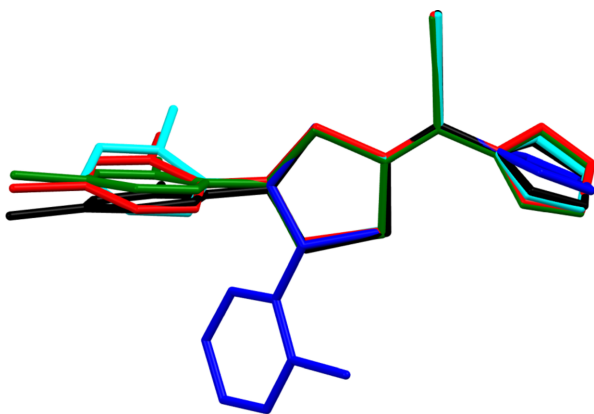
1 - dithiolane ring; 2 - imidazole ring; 3 - dichlorophenyl ring (A and B are the disordered components).

	1/2	1/3	2/3
LCZ-A	62.7 (1)	88.7 (3)	28.4 (3)
LCZ-B	62.7 (1)	74.0 (3)	46.6 (3)
LCZ-opt	81.4	75.2	36.9

group $P2_1$ with one molecule in the asymmetric unit. The LCZ molecule has an *R* configuration at the asymmetric center of atom C8. The dithiolane ring adopts an envelope conformation with the C8 flap atom having a maximum deviation of 0.287 (2) Å, and puckering parameters (Cremer & Pople, 1975) $Q = 0.438$ (2) Å and $\varphi = 295.6$ (3) $^{\circ}$. According to the asymmetry parameters (Duax & Norton, 1975), the mirror plane passes through atom C8 and the C6—S1 bond; $\Delta C_s(C8) = 10.21$ (2) $^{\circ}$. In the LCZ structure, the dichlorophenyl ring was found to be disordered over two orientations and the occupancies of the disordered atoms were fixed at 0.5. Fig. 2 presents an overlay of three independent luliconazole skeletons, considering separately the two disordered components A and B of LCZ, i.e. LCZ-A (red), LCZ-B (green) and the theoretically obtained optimized structure (LCZ-opt, black).

**Figure 1**

The molecular structure of LCZ with the atom-numbering scheme. The disordered components A and B of the dichlorophenyl ring have equal site-occupancies (1/2). Component A is drawn using unbroken lines while component B is drawn using dashed lines without labels. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

**Figure 2**

An overlay of three luliconazole molecules LCZ-A (red), LCZ-B (green), LCZ-opt (black), and two related structures PESWAM (cyan) and DELYAV (blue).

Table 2Hydrogen-bond geometry (Å, $^{\circ}$).

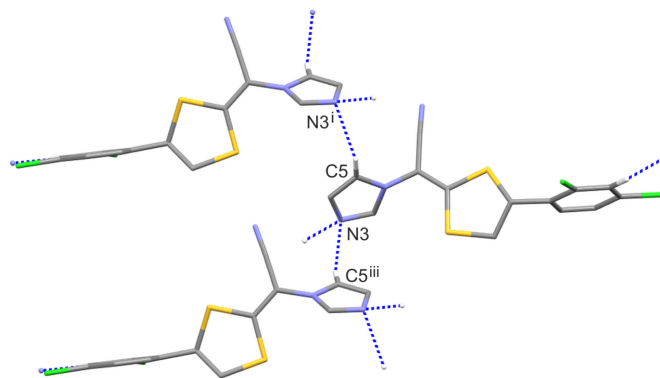
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5\cdots N3^i$	0.93	2.49	3.335 (4)	151
$C11A-H11A\cdots N3^{ii}$	0.93	2.45	3.371 (6)	172
$C11B-H11B\cdots N3^{ii}$	0.93	2.58	3.440 (6)	154

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

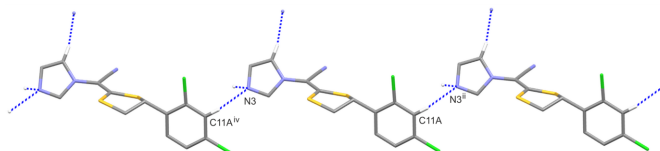
The molecular conformations are quite similar, differing only slightly in the orientations of the imidazole and dichlorophenyl rings. The dihedral angle between the disordered dichlorophenyl rings A and B of LCZ is 18.2 (4) $^{\circ}$. The imidazole ring is planar (r.m.s. deviation = 0.002 Å). The mutual arrangement of the rings can be analyzed by the dihedral angles between their best planes, calculated using the least-squares method (Table 1).

3. Supramolecular features

In the crystal structure of luliconazole, there are no potential strong proton donors, apart from weak C—H bonds. There are two intermolecular hydrogen bonds: $C5-H5\cdots N3(-x, y + \frac{1}{2}, -z + 1)$ and $C11A-H11A\cdots N3(-x, y + \frac{1}{2}, -z + 1)$; in both, the N3 atom is a hydrogen-bond acceptor. The geometric parameters of these interactions are presented in Table 2. Fig. 3 demonstrates that the former interaction produces a mono-periodic chain along the *b*-axis direction, whose first-

**Figure 3**

A part of the crystal structure of LCZ (only disordered component A is shown) showing the formation of the C(4) chain motif. Hydrogen bonds are drawn as dashed lines, and for the sake of clarity, the H atoms not involved in hydrogen bonds have been omitted. Symmetry codes: (i) $-x, y + \frac{1}{2}, -z$; (iii) $-x, y - \frac{1}{2}, -z + 1$.

**Figure 4**

A part of the crystal structure of LCZ (only disordered component A is shown) showing the formation of the C(11) chain motif. Hydrogen bonds are drawn as dashed lines, and for the sake of clarity, the H atoms not involved in hydrogen bonds have been omitted. Symmetry codes: (ii) $x + 1, y, z + 1$; (iv) $x - 1, y, z - 1$.

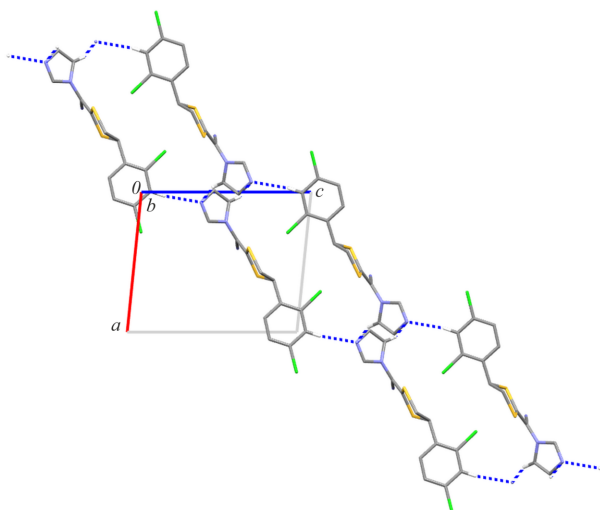


Figure 5
Partial crystal packing of LCZ-A showing the formation of molecular layers parallel to (101).

level graph-set descriptor is $C(4)$ (Etter, 1990; Etter *et al.*, 1990; Bernstein *et al.*, 1995), while the latter interaction generates a $C(11)$ chain motif along the [101] direction (Fig. 4). The combination of these two chain motifs leads to the formation of di-periodic molecular layers parallel to (101) (Fig. 5).

4. Hirshfeld surface analysis

Hirshfeld surfaces and fingerprint plots (Spackman & McKinnon, 2002; Spackman & Jayatilaka, 2009) were generated using *CrystalExplorer* software (Spackman *et al.*, 2021). Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) complements the comparison of the two disordered components of the luliconazole molecule. Fig. 6 presents a comparison of the Hirshfeld surfaces of the LCZ-A and LCZ-B structures and the corresponding 2D fingerprint plots of the most dominant contacts combined with their percentage contributions to the Hirshfeld surface. Red spots on the Hirshfeld surfaces indicate atoms participating in the $C-H\cdots N$ hydrogen bonds and an $N\cdots S$ contact shorter than the sum of their van der Waals radii.

For both molecules, the $H\cdots N/N\cdots H$, $H\cdots Cl/Cl\cdots H$, $H\cdots H$ and $C\cdots H/H\cdots C$ contacts provide the greatest contribution (each about 15–20%) to the Hirshfeld surface. The $H\cdots S/S\cdots H$ interactions contribute about 9%. Other contacts do not exceed 5%. Two pairs of spikes in the $H\cdots N/N\cdots H$ fingerprint plots belong to the closest $N\cdots H$ contacts, while $H\cdots S/S\cdots H$ interactions lead to characteristic sharp spikes for LCZ-A compared to the chicken-wing-like features for LCZ-B.

5. Database survey

A search of the Cambridge Structural Database (CSD version 5.45, June 2024, Groom *et al.*, 2016) did not reveal any struc-

ture of luliconazole. However, two isomeric structures (*E* and *Z*) were found (DELYAV; Lin *et al.*, 2006; PESWAM; Xiao *et al.*, 2006), which differ from luliconazole by the presence of a 2-chlorophenyl ring instead of the dichlorophenyl ring in LCZ. Fig. 2 shows the superposition of their skeletons compared to three luliconazole molecules. PESWAM (isomer *E*) is closely related in molecular conformation to LCZ-A, in contrast to the structure of DELYAV, which differs from the others in the site of substitution (atom C7 vs C8 of the dithiolane ring; isomer *Z*) and the spatial orientation of imidazole ring.

6. Synthesis and crystallization

The luliconazole (purity 98%) used in this study was purchased from BLD Pharmatech GmbH (Germany). A pure crystalline form of luliconazole was obtained unexpectedly from cocrystallization of the drug with pyrazinedicarboxylic acid; all substances (0.05 mmol) were used with a fixed stoichiometric ratio of 1:1, dissolved in ethanol (3 ml EtOH) and the mixture was heated to 346 K.

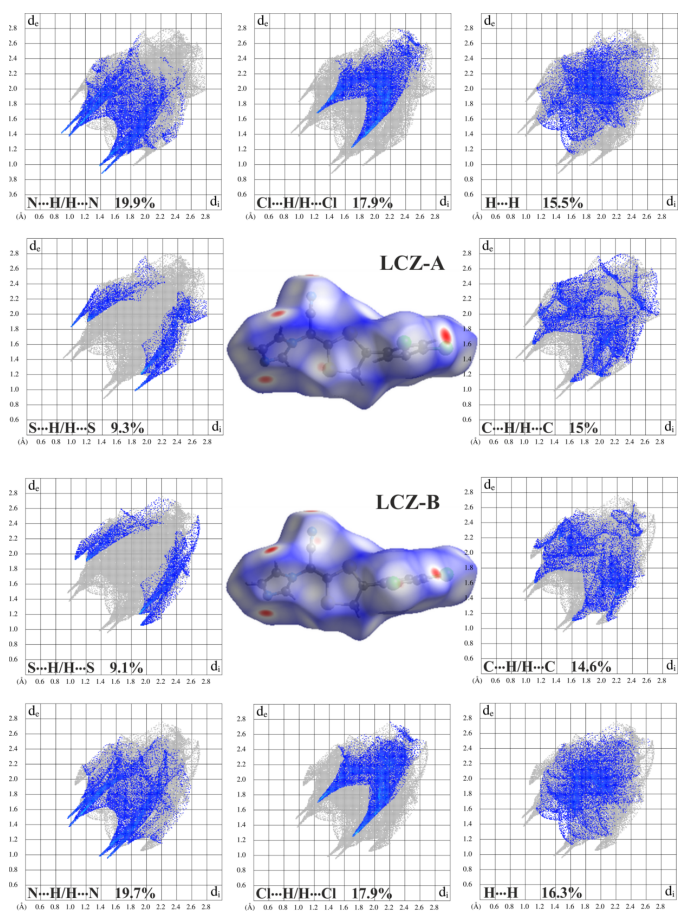


Figure 6
Comparison of Hirshfeld surfaces and the corresponding two-dimensional fingerprint plots of the most dominant contacts for the two disordered components of LCZ (top half for LCZ-A, bottom half for LCZ-B). The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Table 3

Experimental details.

Crystal data	
Chemical formula	C ₁₄ H ₉ Cl ₂ N ₃ S ₂
<i>M_r</i>	354.26
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁
Temperature (K)	294
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.0136 (1), 8.1561 (1), 10.8718 (1)
β (°)	95.778 (1)
<i>V</i> (Å ³)	795.19 (2)
<i>Z</i>	2
Radiation type	Cu <i>K</i> α
μ (mm ^{−1})	6.09
Crystal size (mm)	0.20 × 0.07 × 0.03
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian (<i>CrysAlis PRO</i> ; Rigaku OD, 2023)
<i>T</i> _{min} , <i>T</i> _{max}	0.167, 0.787
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	14902, 3132, 3031
<i>R</i> _{int}	0.026
(<i>sin</i> θ / λ) _{max} (Å ^{−1})	0.632
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.025, 0.069, 1.07
No. of reflections	3132
No. of parameters	238
No. of restraints	295
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ^{−3})	0.15, −0.19
Absolute structure	Flack <i>x</i> determined using 1322 quotients [(<i>I</i> ⁺) − (<i>I</i> [−])]/[(<i>I</i> ⁺) + (<i>I</i> [−])] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	−0.010 (6)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

During the refinement of compound LCZ, the dichlorophenyl ring was found to be disordered over two orientations (ring 1A: C9A, C10A, C11A, C12A, C13A, C14A, C11A, C12A and ring 1B: C9B, C10B, C11B, C12B, C13B, C14B, C11B, C12B); finally site occupancies of two components were fixed at 0.5. Two components of the disorder were modelled, using rigid planar hexagons for the phenyl rings. Furthermore, similarity restraints were applied to the atomic displacement parameters of all disordered atoms using SIMU and ISOR commands in *SHELXL*. The distances between atom pairs C—Cl were restrained to be equal, with an effective s.u. of 0.003 Å.

All hydrogen atoms bonded to carbon atoms were placed geometrically and refined as riding, with *U*_{iso}(H) = 1.2 *U*_{eq}(C) for the methylene, methine and aromatic groups.

8. Theoretical calculations

To make a comparison between the experimental and theoretical models of luliconazole, full geometry optimization of the luliconazole molecule was carried out using *GAUS-*

SIANI6 (Frisch *et al.*, 2019) at the B3LYP/6-311++G(3df,3pd) level of theory. The input coordinates for density functional theory (DFT) calculations were generated from the experimental Cartesian coordinates of the LCZ-A structure. A stationary point of the theoretical model of luliconazole (LCZ-opt) was confirmed by the absence of imaginary frequencies. Cartesian coordinates (XYZ) for the LCZ-opt structure are given in Table S1 in the supporting information.

Acknowledgements

The financial support from University of Lodz Doctoral School of Exact and Natural Sciences is gratefully acknowledged.

References

- Bernstein, J., Davis, R. E., Shimon, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
- Deepshikha, K. & Subhash, B. (2014). *Dovepress*, **9**, 113–124.
- Duax, W. L. & Norton, D. A. (1975). In *Atlas of Steroid Structures*, Vol. 1. New York: Plenum Press.
- Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
- Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* **B46**, 256–262.
- Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A. V., Bloino, J., Janesko, B. G., Gomperts, R., Mennucci, B., Hratchian, H. P., Ortiz, J. V., Izmaylov, A. F., Sonnenberg, J. L., Williams-Young, D., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V. G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery, J. A. Jr, Peralta, J. E., Ogliaro, F., Bearpark, M. J., Heyd, J. J., Brothers, E. N., Kudin, K. N., Staroverov, V. N., Keith, T. A., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A. P., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Millam, J. M., Klene, M., Adamo, C., Cammi, R., Ochterski, J. W., Martin, R. L., Morokuma, K., Farkas, O., Foresman, J. B. & Fox, D. J. (2019). *GAUSSIAN16*. Revision C.02. Gaussian Inc., Wallingford, CT, USA. <https://gaussian.com/>.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Koga, H., Nanjoh, Y., Kaneda, H., Yamaguchi, H. & Tsuboi, R. (2012). *Antimicrob. Agents Chemother.* **56**, 3138–3143.
- Lin, Y., Xiao, T. & Wang, J.-T. (2006). *Acta Cryst.* **E62**, o3159–o3160.
- Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
- Niwan, Y., Kuzuhara, N., Kodama, H., Yoshida, M., Miyazaki, T. & Yamaguchi, H. (1998). *Antimicrob. Agents Chemother.* **42**, 967–970.
- Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* **B69**, 249–259.
- Rigaku OD (2023). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.
- Spackman, M. A. & McKinnon, J. J. (2002). *CrystEngComm*, **4**, 378–392.

- Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
- Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Xiao, T., Lin, Y., Zhang, X.-Q., Chen, J. & Wang, J.-T. (2006). *Acta Cryst.* **E62**, o5052–o5053.

supporting information

Acta Cryst. (2025). E81, 24–28 [https://doi.org/10.1107/S2056989024011812]

Crystal structure of luliconazole

Anna Ben and Lilianna Chęcińska

Computing details

(E)-[(4*R*)-4-(2,4-Dichlorophenyl)-1,3-dithiolan-2-ylidene](1*H*-imidazol-1-yl)acetonitrile

Crystal data

C₁₄H₉Cl₂N₃S₂

M_r = 354.26

Monoclinic, *P*2₁

a = 9.0136 (1) Å

b = 8.1561 (1) Å

c = 10.8718 (1) Å

β = 95.778 (1)°

V = 795.19 (2) Å³

Z = 2

F(000) = 360

D_x = 1.480 Mg m⁻³

Cu *Kα* radiation, λ = 1.54184 Å

Cell parameters from 12732 reflections

θ = 4.1–76.6°

μ = 6.09 mm⁻¹

T = 294 K

Prism, colourless

0.20 × 0.07 × 0.03 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix
diffractometer

Radiation source: micro-focus sealed X-ray
tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: gaussian
(CrysAlisPro; Rigaku OD, 2023)

*T*_{min} = 0.167, *T*_{max} = 0.787

14902 measured reflections

3132 independent reflections

3031 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.026

θ_{max} = 77.2°, θ_{min} = 4.1°

h = −11→10

k = −9→10

l = −13→13

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.025

wR(*F*²) = 0.069

S = 1.07

3132 reflections

238 parameters

295 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F_o*²) + (0.0399*P*)² + 0.0887*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.001

Δρ_{max} = 0.15 e Å⁻³

Δρ_{min} = −0.19 e Å⁻³

Absolute structure: Flack *x* determined using
1322 quotients [(*F*⁺)(*F*)]/[(*F*⁺)(*F*)] (Parsons *et al.*, 2013)

Absolute structure parameter: −0.010 (6)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cl1A	0.7112 (8)	0.3287 (9)	1.1135 (7)	0.0901 (16)	0.5
Cl2A	1.2841 (5)	0.2715 (10)	1.0208 (5)	0.0882 (15)	0.5
Cl1B	0.7057 (9)	0.2672 (10)	1.1114 (7)	0.114 (3)	0.5
Cl2B	1.2743 (5)	0.3102 (11)	1.0307 (6)	0.105 (2)	0.5
S1	0.39907 (7)	0.21429 (7)	0.66512 (6)	0.05387 (17)	
S2	0.59952 (8)	0.49155 (9)	0.73496 (7)	0.0642 (2)	
N1	0.4012 (3)	0.8370 (3)	0.6007 (3)	0.0670 (6)	
N2	0.2121 (2)	0.4772 (3)	0.51520 (18)	0.0454 (4)	
N3	0.0737 (3)	0.3647 (3)	0.3584 (2)	0.0658 (7)	
C1	0.3416 (2)	0.5289 (3)	0.5913 (2)	0.0436 (5)	
C2	0.3726 (3)	0.6999 (3)	0.5944 (2)	0.0488 (5)	
C3	0.2085 (3)	0.3786 (3)	0.4141 (2)	0.0531 (6)	
H3	0.291839	0.327232	0.387726	0.064*	
C4	−0.0127 (3)	0.4596 (4)	0.4260 (3)	0.0724 (9)	
H4	−0.114889	0.473964	0.407721	0.087*	
C5	0.0686 (3)	0.5297 (4)	0.5224 (3)	0.0615 (7)	
H5	0.034806	0.599083	0.581389	0.074*	
C6	0.4336 (3)	0.4234 (3)	0.6568 (2)	0.0454 (5)	
C7	0.5759 (3)	0.1646 (4)	0.7514 (3)	0.0624 (7)	
H7A	0.564313	0.069235	0.802923	0.075*	
H7B	0.649020	0.138719	0.694683	0.075*	
C8	0.6294 (3)	0.3087 (4)	0.8315 (2)	0.0559 (6)	
H8	0.566602	0.317007	0.899744	0.067*	
C9A	0.7953 (5)	0.2935 (9)	0.8872 (7)	0.0553 (13)	0.5
C10A	0.8435 (7)	0.3149 (11)	1.0117 (7)	0.0556 (14)	0.5
C11A	0.9949 (8)	0.3097 (11)	1.0515 (5)	0.0628 (14)	0.5
H11A	1.027154	0.324001	1.134743	0.075*	0.5
C12A	1.0981 (5)	0.2832 (9)	0.9668 (7)	0.0683 (14)	0.5
C13A	1.0499 (6)	0.2618 (8)	0.8423 (6)	0.0619 (14)	0.5
H13A	1.118888	0.244023	0.785627	0.074*	0.5
C14A	0.8985 (7)	0.2670 (7)	0.8025 (5)	0.0579 (14)	0.5
H14A	0.866205	0.252683	0.719235	0.069*	0.5
C9B	0.7923 (5)	0.3066 (9)	0.8760 (7)	0.0528 (13)	0.5
C10B	0.8287 (7)	0.2829 (11)	1.0020 (7)	0.0566 (14)	0.5
C11B	0.9773 (8)	0.2807 (11)	1.0507 (5)	0.0646 (14)	0.5
H11B	1.001705	0.264790	1.135003	0.077*	0.5
C12B	1.0895 (5)	0.3021 (9)	0.9733 (7)	0.0632 (13)	0.5
C13B	1.0531 (6)	0.3258 (8)	0.8473 (7)	0.0648 (14)	0.5
H13B	1.128176	0.340176	0.795514	0.078*	0.5

C14B	0.9045 (7)	0.3281 (8)	0.7986 (5)	0.0602 (14)	0.5
H14B	0.880120	0.343952	0.714286	0.072*	0.5

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1A	0.0641 (16)	0.161 (4)	0.0466 (17)	0.009 (2)	0.0115 (11)	−0.013 (2)
Cl2A	0.0450 (13)	0.138 (4)	0.0786 (16)	0.0186 (15)	−0.0057 (10)	0.023 (2)
Cl1B	0.0780 (18)	0.213 (7)	0.051 (2)	−0.003 (3)	0.0122 (15)	0.034 (3)
Cl2B	0.0491 (16)	0.142 (4)	0.116 (3)	0.0239 (15)	−0.0284 (15)	−0.0304 (19)
S1	0.0493 (3)	0.0458 (3)	0.0639 (4)	−0.0038 (3)	−0.0072 (3)	0.0024 (3)
S2	0.0528 (3)	0.0561 (4)	0.0776 (5)	−0.0055 (3)	−0.0234 (3)	−0.0048 (3)
N1	0.0606 (14)	0.0490 (14)	0.0923 (18)	−0.0040 (11)	0.0118 (12)	−0.0051 (13)
N2	0.0347 (9)	0.0481 (11)	0.0521 (10)	−0.0016 (8)	−0.0012 (7)	−0.0022 (9)
N3	0.0610 (14)	0.0669 (16)	0.0645 (13)	−0.0120 (12)	−0.0180 (11)	0.0023 (11)
C1	0.0375 (11)	0.0453 (12)	0.0470 (11)	−0.0013 (9)	−0.0008 (9)	−0.0052 (9)
C2	0.0405 (11)	0.0481 (14)	0.0571 (13)	0.0033 (10)	0.0020 (9)	−0.0043 (11)
C3	0.0491 (13)	0.0576 (15)	0.0515 (13)	−0.0072 (11)	−0.0005 (10)	−0.0060 (11)
C4	0.0409 (13)	0.0672 (19)	0.104 (2)	−0.0011 (13)	−0.0176 (14)	0.0105 (17)
C5	0.0413 (13)	0.0551 (15)	0.087 (2)	0.0060 (11)	0.0015 (13)	−0.0022 (13)
C6	0.0436 (12)	0.0457 (12)	0.0461 (12)	−0.0020 (10)	−0.0004 (9)	−0.0065 (10)
C7	0.0556 (15)	0.0583 (17)	0.0700 (18)	0.0077 (12)	−0.0101 (13)	0.0066 (13)
C8	0.0441 (12)	0.0763 (18)	0.0460 (11)	0.0081 (13)	−0.0016 (9)	0.0004 (13)
C9A	0.047 (2)	0.077 (3)	0.042 (2)	0.006 (2)	0.002 (2)	0.003 (2)
C10A	0.050 (2)	0.076 (3)	0.039 (2)	−0.001 (2)	−0.005 (2)	−0.003 (2)
C11A	0.051 (2)	0.086 (3)	0.047 (2)	0.002 (2)	−0.013 (2)	−0.001 (2)
C12A	0.053 (2)	0.089 (3)	0.061 (2)	0.009 (2)	−0.005 (2)	0.003 (2)
C13A	0.048 (2)	0.081 (3)	0.057 (2)	0.013 (2)	0.0042 (19)	−0.002 (3)
C14A	0.050 (2)	0.078 (3)	0.045 (2)	0.008 (2)	0.0013 (18)	0.001 (2)
C9B	0.046 (2)	0.075 (3)	0.035 (2)	0.011 (2)	−0.0074 (19)	0.004 (2)
C10B	0.050 (2)	0.079 (3)	0.040 (2)	−0.001 (2)	−0.002 (2)	−0.004 (2)
C11B	0.055 (3)	0.088 (3)	0.048 (2)	0.000 (2)	−0.006 (2)	0.005 (2)
C12B	0.042 (2)	0.087 (3)	0.058 (2)	0.016 (2)	−0.006 (2)	0.001 (2)
C13B	0.049 (2)	0.085 (3)	0.060 (2)	0.010 (3)	0.005 (2)	−0.001 (3)
C14B	0.052 (2)	0.080 (3)	0.048 (2)	0.008 (3)	0.0025 (19)	0.006 (3)

Geometric parameters ($\text{\AA}$, $^\circ$)

Cl1A—C10A	1.711 (3)	C7—H7B	0.9700
Cl2A—C12A	1.722 (3)	C8—C9B	1.499 (5)
Cl1B—C10B	1.710 (3)	C8—C9A	1.561 (5)
Cl2B—C12B	1.720 (3)	C8—H8	0.9800
S1—C6	1.737 (3)	C9A—C10A	1.3900
S1—C7	1.812 (3)	C9A—C14A	1.3900
S2—C6	1.736 (2)	C10A—C11A	1.3900
S2—C8	1.828 (3)	C11A—C12A	1.3900
N1—C2	1.148 (4)	C11A—H11A	0.9300
N2—C3	1.360 (3)	C12A—C13A	1.3900

N2—C5	1.371 (3)	C13A—C14A	1.3900
N2—C1	1.425 (3)	C13A—H13A	0.9300
N3—C3	1.306 (3)	C14A—H14A	0.9300
N3—C4	1.364 (4)	C9B—C10B	1.3900
C1—C6	1.348 (3)	C9B—C14B	1.3900
C1—C2	1.422 (4)	C10B—C11B	1.3900
C3—H3	0.9300	C11B—C12B	1.3900
C4—C5	1.344 (4)	C11B—H11B	0.9300
C4—H4	0.9300	C12B—C13B	1.3900
C5—H5	0.9300	C13B—C14B	1.3900
C7—C8	1.512 (4)	C13B—H13B	0.9300
C7—H7A	0.9700	C14B—H14B	0.9300
C6—S1—C7	95.38 (13)	C10A—C9A—C14A	120.0
C6—S2—C8	95.13 (12)	C10A—C9A—C8	124.2 (5)
C3—N2—C5	106.5 (2)	C14A—C9A—C8	115.7 (5)
C3—N2—C1	126.6 (2)	C11A—C10A—C9A	120.0
C5—N2—C1	126.6 (2)	C11A—C10A—C11A	121.8 (6)
C3—N3—C4	104.8 (2)	C9A—C10A—C11A	117.9 (5)
C6—C1—C2	120.3 (2)	C10A—C11A—C12A	120.0
C6—C1—N2	122.8 (2)	C10A—C11A—H11A	120.0
C2—C1—N2	116.8 (2)	C12A—C11A—H11A	120.0
N1—C2—C1	177.5 (3)	C13A—C12A—C11A	120.0
N3—C3—N2	111.8 (2)	C13A—C12A—C12A	121.5 (5)
N3—C3—H3	124.1	C11A—C12A—C12A	118.4 (5)
N2—C3—H3	124.1	C12A—C13A—C14A	120.0
C5—C4—N3	111.4 (2)	C12A—C13A—H13A	120.0
C5—C4—H4	124.3	C14A—C13A—H13A	120.0
N3—C4—H4	124.3	C13A—C14A—C9A	120.0
C4—C5—N2	105.4 (3)	C13A—C14A—H14A	120.0
C4—C5—H5	127.3	C9A—C14A—H14A	120.0
N2—C5—H5	127.3	C10B—C9B—C14B	120.0
C1—C6—S2	120.55 (19)	C10B—C9B—C8	116.5 (5)
C1—C6—S1	123.39 (19)	C14B—C9B—C8	123.5 (5)
S2—C6—S1	116.03 (14)	C11B—C10B—C9B	120.0
C8—C7—S1	109.7 (2)	C11B—C10B—C11B	113.7 (6)
C8—C7—H7A	109.7	C9B—C10B—C11B	126.2 (6)
S1—C7—H7A	109.7	C10B—C11B—C12B	120.0
C8—C7—H7B	109.7	C10B—C11B—H11B	120.0
S1—C7—H7B	109.7	C12B—C11B—H11B	120.0
H7A—C7—H7B	108.2	C11B—C12B—C13B	120.0
C9B—C8—C7	115.0 (4)	C11B—C12B—C12B	121.5 (5)
C7—C8—C9A	113.5 (3)	C13B—C12B—C12B	118.4 (5)
C9B—C8—S2	106.1 (3)	C14B—C13B—C12B	120.0
C7—C8—S2	106.49 (17)	C14B—C13B—H13B	120.0
C9A—C8—S2	111.6 (3)	C12B—C13B—H13B	120.0
C7—C8—H8	108.4	C13B—C14B—C9B	120.0
C9A—C8—H8	108.4	C13B—C14B—H14B	120.0

S2—C8—H8	108.4	C9B—C14B—H14B	120.0
C3—N2—C1—C6	−62.6 (4)	C14A—C9A—C10A—C11A	0.0
C5—N2—C1—C6	124.2 (3)	C8—C9A—C10A—C11A	−175.7 (6)
C3—N2—C1—C2	116.4 (3)	C14A—C9A—C10A—C11A	−174.2 (7)
C5—N2—C1—C2	−56.8 (4)	C8—C9A—C10A—C11A	10.0 (6)
C4—N3—C3—N2	0.6 (3)	C9A—C10A—C11A—C12A	0.0
C5—N2—C3—N3	−0.5 (3)	C11A—C10A—C11A—C12A	174.0 (7)
C1—N2—C3—N3	−174.8 (2)	C10A—C11A—C12A—C13A	0.0
C3—N3—C4—C5	−0.4 (4)	C10A—C11A—C12A—C12A	−178.1 (6)
N3—C4—C5—N2	0.1 (4)	C11A—C12A—C13A—C14A	0.0
C3—N2—C5—C4	0.2 (3)	C12A—C12A—C13A—C14A	178.0 (6)
C1—N2—C5—C4	174.5 (3)	C12A—C13A—C14A—C9A	0.0
C2—C1—C6—S2	−5.7 (3)	C10A—C9A—C14A—C13A	0.0
N2—C1—C6—S2	173.31 (18)	C8—C9A—C14A—C13A	176.1 (6)
C2—C1—C6—S1	176.36 (19)	C7—C8—C9B—C10B	−111.8 (4)
N2—C1—C6—S1	−4.7 (3)	S2—C8—C9B—C10B	130.8 (3)
C8—S2—C6—C1	164.4 (2)	C7—C8—C9B—C14B	68.7 (6)
C8—S2—C6—S1	−17.54 (17)	S2—C8—C9B—C14B	−48.7 (5)
C7—S1—C6—C1	174.3 (2)	C14B—C9B—C10B—C11B	0.0
C7—S1—C6—S2	−3.76 (18)	C8—C9B—C10B—C11B	−179.5 (6)
C6—S1—C7—C8	29.9 (2)	C14B—C9B—C10B—C11B	175.7 (7)
S1—C7—C8—C9B	−161.5 (4)	C8—C9B—C10B—C11B	−3.8 (7)
S1—C7—C8—C9A	−167.4 (4)	C9B—C10B—C11B—C12B	0.0
S1—C7—C8—S2	−44.3 (2)	C11B—C10B—C11B—C12B	−176.2 (7)
C6—S2—C8—C9B	159.7 (3)	C10B—C11B—C12B—C13B	0.0
C6—S2—C8—C7	36.8 (2)	C10B—C11B—C12B—C12B	176.8 (7)
C6—S2—C8—C9A	161.1 (3)	C11B—C12B—C13B—C14B	0.0
C7—C8—C9A—C10A	−129.6 (4)	C12B—C12B—C13B—C14B	−176.9 (6)
S2—C8—C9A—C10A	110.0 (4)	C12B—C13B—C14B—C9B	0.0
C7—C8—C9A—C14A	54.5 (5)	C10B—C9B—C14B—C13B	0.0
S2—C8—C9A—C14A	−65.9 (5)	C8—C9B—C14B—C13B	179.5 (6)

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
C5—H5 $\cdots$ N3 ⁱ	0.93	2.49	3.335 (4)	151
C11A—H11A $\cdots$ N3 ⁱⁱ	0.93	2.45	3.371 (6)	172
C11B—H11B $\cdots$ N3 ⁱⁱ	0.93	2.58	3.440 (6)	154

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