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Crystal, molecular structure, and conformational preferences of 3-(2-(4-morpholinophenyl)-2-oxoethyl)-5,5-diphenylimidazolidine-2,4-dione

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ABSTRACT

The X-ray crystal structure of 3-(2-(4-morpholinophenyl)-2-oxoethyl)-5,5-diphenylimidazolidine-2,4-dione (**2**) [$C_{27}H_{25}N_3O_4$: MF = 455.50, monoclinic, $P2_1/c$, a = 6.2038 (2) Å, b = 20.8905 (6) Å, c = 18.3361 (6) Å, b = 97.594 (2)°, V = 2355.53 Å^3, Z = 4, D_{calc} = 1.284 Mg m^{-3}, λ = 1.54178 Å] was determined. The crystal packing confirmed the occurrence of two conformers of opposite conformation. Conformational aspects of compound **2** have pointed out two factors that determine the conformation of the system under investigation: first, the intermolecular hydrogen bonding of the crystal packing, which stabilizes and favors the occurrence of two independent molecules, and the second factor is the steric hindrance among substituents.

KEYWORDS

Imidazolidine-2,4-dione; UV-spectra; X-ray crystal structure; crystal pack; conformers

Introduction

Much attention has been given to pharmaceutical organic compounds due to their biological applications [1–7]. The importance of azolidinones, which were defined by nitrogen heteroatomic system, with at least of one carbonyl group is well reported [1, 2, 5–7]. This common template was found in the structures of two well-established imidazolidin-2-one and imidazolidine-2,4-dione (hydantoin) that showed a wide range of biological activity, including their anticonvulsant [8], anticancer [1, 2, 5–7], and carbonic anhydrase inhibiting activities [9]. Due to the biological importance of this class of compounds, their molecular structures are extensively studied by means of spectroscopic and theoretical methods [10–16]. Moreover, urea molecule, which is the main core of imidazolidin-2-one and imidazolidine-2,4-dione, have been one of the most thoroughly investigated systems, experimentally as well as theoretically. It contains NH and CO groups, which provide a wide range of possible hydrogen bonds between the adjacent urea molecules in the crystal [17–22]. The crystal form of urea showed

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a planar conformation [17–22], which mainly related to the existence of an extensive network of hydrogen bonds [23].

In the present study, the X-ray analysis of 3-(2-(4-morpholinophenyl)-2-oxoethyl)-5,5-diphenylimidazolidine-2,4-dione (**2**) has been performed, focusing on the configuration of substituents around the imidazolidine-2,4-dione core. The spectroscopic interpretation of the title compound **2** based on Fourier transform–Infrared spectroscopy (FT-IR) and Ultraviolet–Visible (UV-Vis) spectral analysis has been carried out. Molecular electrostatic potential (MEP) has been used for understanding hydrogen bonding interactions in the crystal pack.

Experimental

Chemistry

Compound **2** was prepared according to our previous report [7]. UV-Vis analysis was performed with UV spectrophotometer model UV-1800 from Shimadzu Corporation, Kyoto, Japan. It is equipped with 1-cm-matched quartz cells, and the spectra were recorded using a computer-assisted software. Melting points (uncorrected) were recorded on Barnstead 9100 Electrothermal melting apparatus. Infrared (IR) spectra were recorded on an FT-IR Perkin-Elmer spectrometer. ^{1}H NMR were recorded in DMSO-d_6 on Bruker 500 MHz instruments using tetramethylsilane (TMS) as an internal standard (chemical shifts in d ppm), and ^{13}C NMR were recorded in DMSO-d_6 on Bruker 125 MHz instruments using TMS as internal standard (chemical shifts in d ppm). X-ray crystallography was determined using Bruker APEX-II CCD diffractometer. Crystallographic data of 3-(2-(4-morpholinophenyl)-2-oxoethyl)-5,5-diphenylimidazolidine-2,4-dione (**2**) have been deposited with the Cambridge Crystallographic Data Centre (it may be obtained on request quoting the deposition number CCDC 924043 from the CCDC, 12 Union Road, Cambridge CB21EZ, UK. Torsion angles, bond distances, and bond angles are deposited as supplementary material. Fax: 44-01223-336-033; E-mail: deposit@ccdc.cam.ac.uk).

UV-Vis methodology

Stock solution containing 1 mg/mL of compound **2** was prepared in methanol or dichloromethane and 0.2 mL of each stock solution was diluted to 10 mL with each solvent to obtain solution containing 20 mg/mL of each solvent. Each solution was recorded versus the corresponding solvent as a blank.

X-ray crystal structure determination

Procedure for single crystals formation

The pure single crystal of compound **2** was taken from methanol heated with stirring till it dissolved the crude compound, filtered while hot in 25-mL conical flask using filter paper. The flask was corked and kept for a day. The crystals were formed by slow evaporation technique, isolated, and washed with cooled methanol.

Data collection

It was carried out on a Bruker APEX-II CCD diffractometer equipped with a graphite monochromated CuKα radiation, $\lambda = 1.54178$ Å at 296 (2) K. The structure was solved by

direct methods using SHELXS-97 [24]. Data collection: Bruker APEX2 [25]; cell refinement: Bruker SAINT; data reduction: Bruker SAINT [25]; molecular graphics: Bruker SHELXTL; and software used to prepare material for publication: Bruker SHELXTL. A clear colorless block-like specimen of $C_{27}H_{25}N_3O_4$, approximate dimensions 0.62 × 0.17 × 0.17 mm, was used for X-ray crystallographic analysis. The integration of the data using a Monoclinic unit cell, space group $P2_1/c$, yielded a total of 24,834 reflections to a maximum θ angle of 69.7°, of which 4404 were independent (completeness = 98.6%, $R_{int} = 0.044$, $R_{sig} = 0.0392$, and R [$F^2 > 2\sigma(F^2)$] = 0.066. The final cell constants of $a = 6.2038$ (2) Å, $b = 6.2038$ (2) Å, $c = 18.3361$ (6) Å, and volume = 2355.52 (13) Å^3 are based upon the refinement of the XYZ-centroids of 3380 reflections above 20 σ(I) with 6.4° < 2θ < 134.2°. Data were corrected for absorption effects using the multi-scan method (SADABS) [25]. Materials for publication were prepared using PLATON [26] and Mercury [27].

Geometry

All Electrostatic Discharge (ESD) values (except the ESD in the dihedral angle between two Least-squares (LS) planes) are estimated using the full covariance matrix. The cell ESD values 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 ESD involving LS 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*-factor, *R*, is 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. H-atoms attached to carbon were placed in calculated positions (C–H = 0.95–0.98 Å), while those attached to nitrogen were placed in locations derived from a difference map. All were included as riding contributions with isotropic displacement parameters 1.2–1.5 times those of the attached atoms. Friedel opposites were merged in the final refinement.

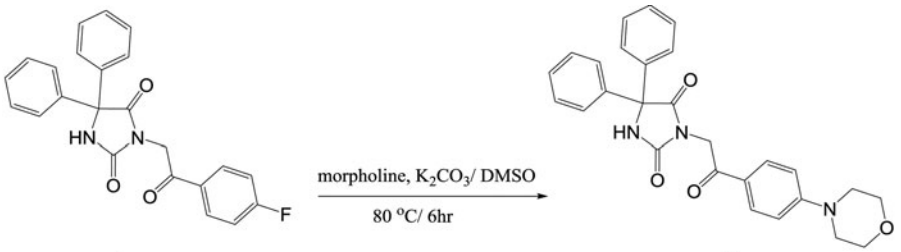
3D-molecular electrostatic potential map

Molecular electrostatic potential was calculated on the optimized structures of both conformers of compound **2** at RM1 [28] level of semi-empirical molecular orbital method using Spartan'14 molecular modeling program [29].

Results and discussion

Chemistry

Compound **2** was prepared according to our previous report by heating compound **1** with morpholine in the presence of K_2CO_3 and DMSO for 6 hr (Scheme 1). The chemical structure of compound **2** was confirmed by nuclear magnetic resonance (NMR), IR, and mass spectral analysis [7].



Scheme 1. Synthesis of 3-(2-(4-morpholinophenyl)-2-oxoethyl)-5,5-diphenylimidazolidine-2,4-dione (**2**) according to Alanazi et al. [7].

UV-Vis and FT-IR Spectra

The UV-Vis and IR spectra of compound **2** are listed in Table 1. The UV-Vis of compound **2** was performed in methanol and dichloromethane, and it showed UV-Vis absorbance bands at the UV region of 327.5 and 328 nm respectively. This band was considered the allowed π-π^* transitions of the aromatic system and the forbidden n-π^* transitions of carbonyl group.

The IR spectrum of compound **2** (Table 1) displays three peaks within the 3176–2831 cm^{-1} region. In this region, there is one stretching vibration of the NH group with the highest peak (3176 cm^{-1}) in the FT-IR spectra. The other two stretching vibrations (2964 and 2831 cm^{-1}) could be detected as CH stretching of aromatic ring and CH_2 stretching of aliphatic moiety. Some bending vibrations were assigned to the CH_2 at 1445 and 1008 cm^{-1} in the FT-IR spectra. The carbon–oxygen (C=O) bands of compound **2** are the most characteristic bands in the vibration spectrum. The C=O stretching vibrations are generally found in the region of 1774–1678 cm^{-1}. In this work, C=O vibration of phenacyl fragment was experimentally measured at 1774 cm^{-1} as a weak band, while the C=O of hydantoin ring vibrated as strong bands at 1717 and 1678 cm^{-1}. In this region, other characteristic peak is the carbon–carbon bond stretching vibrations. C=C stretching vibrations were measured smaller than C=O vibrations. In the FT-IR spectra, 1597 and 1518 cm^{-1} peaks were determined as C=C stretching vibrations. Moreover, C–C and C–O stretching bands were observed at 1490–1377 cm^{-1} and 1192–1112 cm^{-1} respectively.

The single-crystal X-ray analysis of compound 2

The molecular solid-state structure and numbering system of compound **2** are indicated in Figure 1. Crystallographic data, details of the data collection, and structure refinements are listed in Table 2. In the crystal structure of compound **2** (Table 2, Figure 1), it crystallizes with $Z = 4$ in the space group $P2_1/c$ (Table 2).

Table 1. UV-Vis and IR spectra of compound **2**.

UV-Vis (nm, I_{max})		IR (cm^{-1}, n)					
MeOH	CH_2Cl_2	NH Stretching	CH Aromatic stretching	CH Aliphatic stretching	C=O Stretching	C=C Stretching	C-O Stretching
327.5	328.0	3176.4	2964.7	2831.9	1774.8 1717.4 1678.6	1597.4 1518.8	1192.6 1146.11112.6

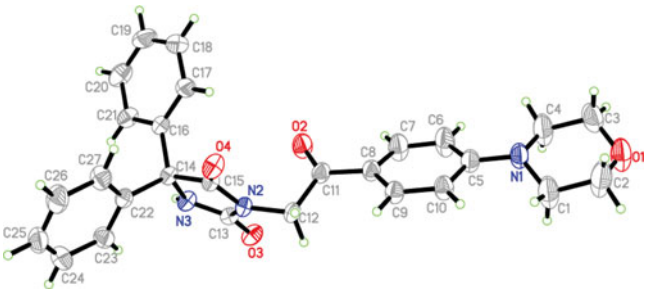


Figure 1. ORTEP drawing of the basic crystallographic unit of compound **2** showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level, and all H atoms are shown as small spheres of arbitrary radii.

Table 2. Experimental X-ray details of structure **2**.

A. Crystal data	
Empirical formula	$C_{27}H_{25}N_3O_4$
Formula weight	455.50
Crystal color, habit	Block, colorless
Crystal dimensions	0.62 × 0.17 × 0.17
Crystal system	Monoclinic
Lattice parameters	a = 6.2038 (2) Å b = 20.8905 (6) Å c = 18.3361 (6) Å β = 97.594 (2)° v = 2355.52 (13) Å
Space group	$P2_1/c$
Z-value	4
D_{calc}	1.284 g cm^{-3}
F_{000}	960
μ (CuKα)	0.71 cm^{-1}
B. Intensity measurements	
Diffractometer	Bruker APEX-II CCD diffractometer
Radiation	CuKα (λ = 1.54178 Å) Graphite monochromated
Detector distance	4.0 mm
Voltage, current	40 kV, 30 mA
Temperature	296 K
Scan type	φ and ω scans
$2\theta_{max}$	134.2°
No. of reflections measured	Total: 24,834 Unique : 4404 (R_{int} = 0.044)
Corrections	multi-scan SADABS Bruker 2009
C. Structure solution and refinement	
Structure solution	Direct methods
Refinement	Full-matrix least-squares
Anomalous dispersion	All non-hydrogen atoms
No. of observations ($I > 2\sigma(I)$)	3380
Residuals: *R*; *Rw*	0.066; 0.198
Residuals *R*1	0.0656
No. of reflections to calc *R*1	3380
Goodness of fit indicator	1.09
Maximum peak in final diff. map	0.69 e^-/Å^3
Minimum peak in final diff. map	−0.41 e^-/Å^3

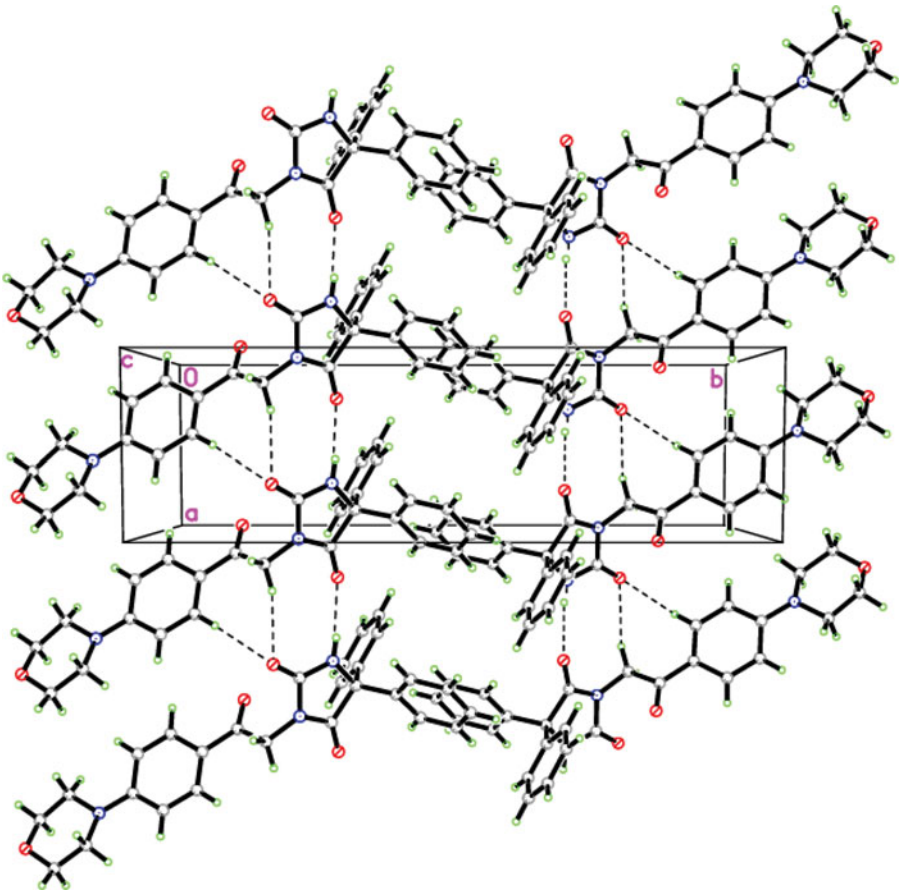


Figure 2. Crystal packing of compound **2** with two conformers **A** (left layer) and **B** (right layer). Hydrogen bonds are shown in dash lines.

The title compound is composed of a central imidazolidine-2,4-dione ring with 5,5-diphenyl moiety and a phenacyl group connected to the N2 of the core ring system. Both 5-phenyl groups are orthogonal and the phenacyl moiety is stabilized in an extended conformation. The crystal packing showed two conformers, which have extended-shape with a different geometry of 5,5-diphenylimidazolidine-2,4-diones and different conformations of phenacyl groups. Recently, crystal structures having more than one molecule in the unit cell can help in understanding the interactions responsible for packing as well as guiding the design of technologically useful materials [30].

As shown in the crystal pack (Figure 2), the two conformers have different conformations as indicated by the dihedral angles between the central imidazolidine-2,4-dione ring A (N3/C14/C15/N2/C13), phenyl ring B (C16–C21), and phenyl ring C (C22–C27) and 2-(4-morpholinophenyl)-2-oxoethyl side chain ring D. In conformer-**A**, these are –1.6° and –112.6° to the phenyl rings based on C16 and C22 respectively, and 74.9° to the 2-(4-morpholinophenyl)-2-oxoethyl side chain. In conformer-**B**, the corresponding angles are 1.6°, 112.6°, and –74.7° respectively (Figures 2 and 3). These disorders are not unexpected due to the conformational flexibility of the 2-(4-morpholinophenyl)-2-oxoethyl side chain and 5,5-diphenyl fragments. In the two conformers (**A** and **B**), the geometrical parameters of the imidazolidine-2,4-dione ring are quite similar (Figures 2 and 3). The geometries of H3-N3-C13 and H3-N3-C14 atoms are almost planar rather than the most stable pyramidal form

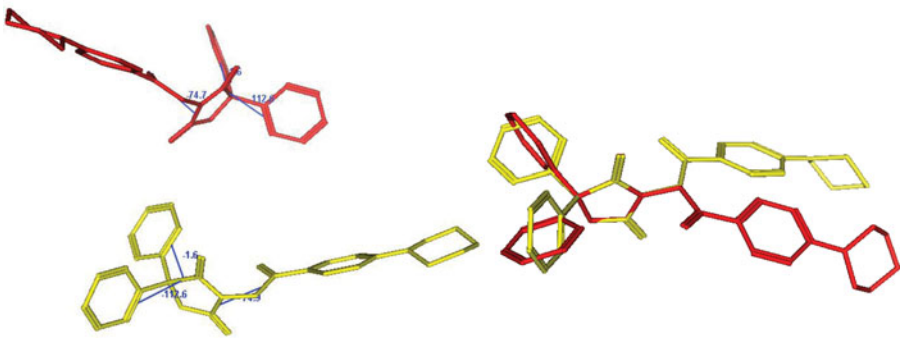


Figure 3. X-ray structures of the two conformers of compound **2** (yellow: conformer-**A** and red: conformer-**B**) retrieved from crystal pack and the superposition of conformers **A** (yellow) and **B** (red).

with bond angles of ca. 121.7° (**A**) and 123° (**B**), and ca. 121.6° (**A**) and 122.1° (**B**) respectively. Similarly, the geometries of C13-N2-C12 and C15-N2-C12 are also planar with bond angles of ca. 122.5° (**A**) and 122.6° (**B**), and 124.2° (**A**) and 124.1° (**B**) respectively [15, 31, 32]. This geometry makes the two nitrogen atoms in each conformer distinguishable from the geometrical point of view. Moreover, the planarity angle ∠N3-C13-N2-C12 of both conformers **A** and **B** was deviated from the planar urea form by 10° with ca 170° [15, 33].

A common characteristic of molecules **A** and **B** is the dihedral angles of 74.9° (**A**) and –74.6° (**B**) between phenacyl group and the imidazolidine-2,4-dione rings; these were expected to minimize unfavorable steric interactions between diketone of the ring system and phenacyl moiety. Another characteristic feature of the two molecules is the relative orientation of phenacyl groups: they adopt an opposite conformation and are nearly out of plane of the corresponding imidazolidine-2,4-dione. In addition, the structures of both conformers **A** and **B** were superimposed by the auto-fit diagram to reveal conformational differences of the two molecules (Figure 3).

The strategy of overlay fit matched imidazolidine-2,4-dione rings and examined any spatial differences between the atoms of peripheral fragments. Moreover, it is obvious from the crystal packing that the molecules are arranged in parallel layers constituted by conformers **A** (Figure 2, left layer) and **B** (Figure 2, right layer) and are maintained by intermolecular classical (NH—O=C) and non-classical (CH_2—O and CH—O) hydrogen bonds, which are likely to be quite enough and an important factor to determine the crystal packing [15, 34].

The main putative interactions NH3—O4=C, as inferred by relatively short distances, wide angle, and suitable orientations, are indicated in Table 3 and Figure 2 [15, 35, 36]. Further, the hydrogen atom H12B of CH_2 of phenacyl moiety and H9A of the aromatic phenacyl ring make bifurcated intermolecular hydrogen bonds with O3 of urea part of the ring system with the bond lengths of 2.4–2.5 Å and bond angles of 154–163°. Finally, it must be indicated that the relative orientation between two parallel molecules of compound **2** in the crystal packing is always 5,5-diphenyl head-to-head, what might indicate, besides steric suitability, a tendency

Table 3. Hydrogen-bond geometry (Å, °).

D—H···A	*d*(D—H)	*d*(H···A)	*d*(D···A)	∠D—H···A
N3—H3N···O4i	0.81 (3)	2.10 (3)	2.906 (2)	170.00 (3)
C9—H9A···O3ii	0.93	2.40	3.264 (3)	154.00
C12H12B···O3ii	0.97	2.50	3.441 (3)	163.00

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

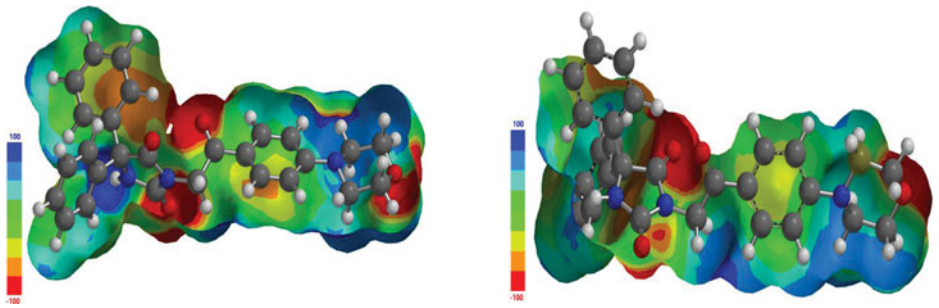


Figure 4. Molecular potential maps of compound **2** for both conformers **A** (left panel) and **B** (right panel).

to minimize the polarity of the crystal (compensating the dipole moments of molecules) [15, 35].

Molecular electrostatic potential contour map

To predict sites of hydrogen bonding and other intermolecular interaction of the two conformers (**A** and **B**) of compound **2**, Molecular electrostatic potential (3D MEP) contour map was calculated on the RM1 semi-empirical level [28] of theory using Spartan'14 molecular modeling program [29] as shown in Figure 4. The surface displays in terms of color grading with red and blue regions refer to the electron rich and electron poor regions, and the green region on the surface suggests almost the neutral region. MEP is formed by the nuclei and the electrons within the molecule [37, 38]. The MEP map shows that the negative potential is on electronegative atoms (electron-rich region), while the positive potential is found around the hydrogen atoms (electron-poor region). These potential gives more information about the region from where the molecule can have intermolecular interactions, especially in crystal packing. Figure 4 shows that the negative charge is located over oxygen atoms to which an electrophile would be strongly attracted and also an indicative of hydrogen bond acceptor. Moreover, the blue regions are located on hydrogen atoms of NH, CH_2, and CH of aromatic ring to which a nucleophile would be attracted and considered as a hydrogen bond donor.

Conclusions

The crystal structures of 3-(2-(4-morpholinophenyl)-2-oxoethyl)-5,5-diphenylimidazolidine -2,4-dione(**2**) has been reported. This compound **2** crystallized in layers formed by crystallographic independent molecules. These crystallographic motifs are the consequence of the interplay of diverse intermolecular interactions (hydrogen bonds) in crystal packing. It is found that the solid-state conformations of the two molecules of **2** (**A** and **B**) in the unit cell are quite different, showing minor differences in some bond length, and major difference in bond angles and torsion angles at peripheral substitution. However, in spite of high congestion in the molecular structures of these two molecules **A** and **B**, they form quite molecular packing that likely reflects the subtle influence of diverse intermolecular interactions. Conformational aspects of compound **2** have pointed out two factors that determine the conformation of the system under investigation. The first one is intermolecular hydrogen bonding of crystal packing such hydrogen bonding stabilizes and favors the occurrence of two independent molecules; and the second factor is steric hindrance between substituents.

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