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Data Article

Single crystal X-ray structural and Hirshfeld surface analysis dataset for some isobutyl-1,2,6-triaryl-4-(arylamino)-1,2,5,6-tetrahydropyridine-3-carboxylates

Chandran Udhaya Kumar[a], Poyyamozhi Surendar Anand[a], Annamalai Sethukumar[a], Kuppusamy Krishnasamy[a], Sivakolunthu Senthan[a], Govindhasamy Manikandan[a,b], Balasubramaniam Arul Prakasam[a,b,*]

[a] Department of Chemistry, Annamalai University, Annamalainagar, Chidambaram 608 002, India
[b] Department of Chemistry, Government Arts College (Autonomous), Kumbakonam 612 002, India

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ABSTRACT

This article reports the single-crystal X-ray diffraction dataset of some isobutyl-1,2,6-triaryl-4-(arylamino)-1,2,5,6-tetrahydropyridine-3-carboxylate (**1-3**) derivatives with Hirshfeld surface analysis. Pictorial representations of intramolecular hydrogen bonding in **1-3** with the characteristics of Resonance Assisted Hydrogen Bonding (RAHB) are presented. The data corresponding to the Hirshfeld surface analysis is given.

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* Corresponding author at: Department of Chemistry, Annamalai University, Annamalainagar, Chidambaram 608 002, India.
E-mail address: arul7777@yahoo.com (B.A. Prakasam).

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Specifications Table

Subject	Organic Chemistry
Specific subject area	Structural Chemistry
Type of data	Figure, Table
How data were acquired	**Single Crystal X-ray diffraction**: Bruker, 2004 APEX 2 diffractometer (for **1** and **3)** and Bruker D8 QUEST diffractometer (for **2**). **Hirshfled**: Crystal Explorer 3.1 version software.
Data format	Raw data and Analyzed.
Parameters for data collection	**SXRD**: Diffraction data were collected on a Bruker, 2004 APEX 2 diffractometer using graphite monochromated Mo Kα radiation ($\lambda = 0.71073$ Å) at 296 K for **1** and **3,** and for **2** Bruker D8 QUEST diffractometer was used with graphite monochromated Mo Kα radiation ($\lambda = 0.71073$ Å) at 100 K. **Hirshfled**: The fingerprint plots and Hirshfeld surface data were generated by using Crystal Explorer 3.1 software program.
Description of data collection	Crystals of compounds were immersed in cryo-oil, mounted in a nylon loop.
Data source location	Department of Chemistry, Annamalai University, Annamalainagar, Chidambaram, 608 002, Tamil Nadu, India.
Data accessibility	Single crystal X-ray structural and Hirshfeld surface analysis data can be accessed at https://data.mendeley.com/datasets/4p5t89zs4v/draft?a=b8bfd08f-a27c-4919-ae70-0648f7ed9116. The Cambridge Crystallographic Data Centre. CCDC 1978944 (for 1), 1978942 (for 2) and 1978943 (for 3), Copies of the data can be obtained free of charge via (http://www.ccdc.cam.ac.uk/conts/retrieving.html, Email: deposit@ccdc.cam.ac.uk.).
Related research article	Poyyamozhi Surendar Anand, Annamalai Sethukumar, Chandran Udhaya Kumar, Kuppusamy Krishnasamy, Sivakolunthu Senthan, Govindhasamy Manikandan, Balasubramaniam Arul Prakasam, Synthesis, stereochemical, single crystal X-ray structural and antimicrobial studies of some isobutyl-1,2,6-triaryl-4-(arylamino)-1,2,5,6-tetrahydropyridine-3-carboxylates: Exploring RAHB with S(6) graph set, J. Mol. Struct. 2020, 129563, https://doi.org/10.1016/j.molstruc.2020.129563.

Value of the Data

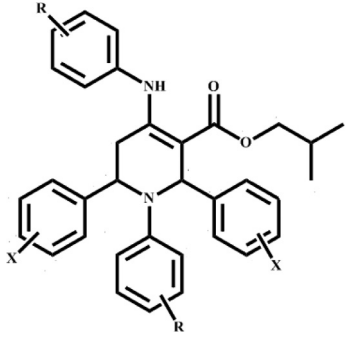
- The presented single crystal X-ray diffraction data will be of interest to researchers in the field of structural chemistry for the comparison with other XRD reports.
- The data will be useful to the researchers who are interested in studying Resonance Assisted Hydrogen Bonding (RAHB).
- The quantified intermolecular interactions in the crystal structures by Hirshfeld surface analysis is the modern approach towards the packing analysis in the crystals.
- The data in this article will be useful for the investigators who are interested in studying non bonded interactions.

1. Data Description

The single crystal X-ray structural data of compounds **1-3** are presented with their Hirshfeld surface analysis in this report. Selected bond distances, bond angles, torsion angles, anisotropic atomic displacement and atomic coordinates for **1-3** are depicted in **Table 1-15**. The molecular structure of the compounds **1-3** are given in **Fig. 1.** The pseudo six-membered rings formed due to Resonance Assisted Hydrogen Bonding (RAHB) are shown in **Fig. 2**. Hirshfeld surface analysis and fingerprint plots were carried out and the intermolecular interactions are quantified [1-8]. Hirshfeld surface mapped with d_{norm}, d_i, d_e, shape index and curvedness of compounds **1, 2,** and **3** are shown in **Fig. 3, 5,** and **7** where, d_{norm} = Normalized contact distance, d_i = Distance

Table 1
Atomic coordinates and equivalent isotropic atomic displacement parameters (Å) for compound **1**.

	x/a	y/b	z/c	U (eq)
C1	0.46891(17)	0.87888(14)	0.64988(13)	0.0565(4)
C2	0.4792(2)	0.85604(18)	0.75671(16)	0.0758(6)
C3	0.4165(2)	0.78351(18)	0.82011(14)	0.0795(7)
C4	0.3432(2)	0.73104(17)	0.77819(14)	0.0745(6)
C5	0.33077(17)	0.75441(15)	0.67094(13)	0.0575(4)
C6	0.39321(13)	0.82940(11)	0.60676(10)	0.0392(3)
C7	0.40657(12)	0.78689(11)	0.42506(10)	0.0350(3)
C8	0.49144(13)	0.66295(11)	0.45111(10)	0.0370(3)
C9	0.60848(13)	0.63552(11)	0.36493(9)	0.0363(3)
C10	0.41857(13)	0.72723(11)	0.25121(10)	0.0355(3)
C11	0.37124(13)	0.81913(11)	0.32429(10)	0.0366(3)
C12	0.32985(12)	0.64689(11)	0.26362(9)	0.0341(3)
C13	0.19476(13)	0.69441(12)	0.25093(12)	0.0436(3)
C14	0.11446(14)	0.62387(12)	0.25639(12)	0.0457(3)
C15	0.16693(14)	0.50315(12)	0.27460(10)	0.0400(3)
C16	0.29973(14)	0.45379(12)	0.28822(11)	0.0421(3)
C17	0.37949(13)	0.52617(11)	0.28238(10)	0.0386(3)
C18	0.1349(2)	0.32154(15)	0.26096(16)	0.0675(5)
C19	0.63647(13)	0.60777(12)	0.17860(10)	0.0376(3)
C20	0.58244(15)	0.60704(14)	0.08635(11)	0.0459(3)
C21	0.66073(17)	0.55173(15)	0.00515(11)	0.0545(4)
C22	0.79407(17)	0.49552(16)	0.01192(12)	0.0579(4)
C23	0.84792(15)	0.49602(15)	0.10179(12)	0.0536(4)
C24	0.77203(14)	0.54988(13)	0.18424(11)	0.0441(3)
C25	0.70710(13)	0.69922(13)	0.37462(10)	0.0402(3)
C26	0.70408(15)	0.80837(14)	0.31754(13)	0.0517(4)
C27	0.78949(17)	0.86769(16)	0.33293(15)	0.0622(4)
C28	0.88021(16)	0.81895(18)	0.40624(14)	0.0605(4)
C29	0.88731(17)	0.70988(19)	0.46244(13)	0.0656(5)
C30	0.80094(15)	0.65038(16)	0.44619(12)	0.0537(4)
C31	1.0489(2)	0.8429(3)	0.4939(2)	0.1061(9)
C32	0.29313(15)	0.93706(12)	0.28857(11)	0.0432(3)
N1	0.55871(10)	0.66221(10)	0.26143(8)	0.0374(3)
N2	0.37621(13)	0.86057(11)	0.49752(9)	0.0430(3)
O1	0.25499(12)	1.01787(9)	0.34048(9)	0.0572(3)
O2	0.26345(13)	0.95158(9)	0.18869(9)	0.0622(3)
O3	0.07968(11)	0.43958(10)	0.27847(9)	0.0568(3)
O4	0.96053(15)	0.88513(15)	0.41546(13)	0.0885(5)
C33	0.1679(18)	1.0666(17)	0.1453(9)	0.089(3)
C34	0.1944(10)	1.0710(8)	0.0289(5)	0.110(3)
C35	0.3327(10)	1.0644(9)	-0.0139(7)	0.176(4)
C36	0.1085(13)	1.1892(9)	-0.0206(8)	0.139(4)



Compound No.	R	X
1	H	*p*-OCH_3
2	F	*p*-OCH_3
3	F	*p*-CH_3

Fig. 1. Molecular structure of compounds **1-3**.

Table 2
Anisotropic atomic displacement parameters (Å) for compound 1.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0664(10)	0.0511(9)	0.0572(9)	-0.0093(7)	-0.0172(8)	-0.0187(8)
C2	0.1018(15)	0.0672(12)	0.0630(11)	-0.0178(10)	-0.0368(11)	-0.0136(11)
C3	0.1127(17)	0.0666(12)	0.0404(9)	-0.0131(8)	-0.0197(10)	0.0086(11)
C4	0.0914(14)	0.0666(11)	0.0486(10)	0.0016(8)	0.0117(9)	-0.0135(10)
C5	0.0637(10)	0.0585(10)	0.0515(9)	-0.0073(7)	0.0014(7)	-0.0235(8)
C6	0.0429(7)	0.0364(7)	0.0357(7)	-0.0100(5)	-0.0026(5)	-0.0060(5)
C7	0.0356(6)	0.0355(7)	0.0348(6)	-0.0058(5)	-0.0012(5)	-0.0124(5)
C8	0.0407(7)	0.0378(7)	0.0302(6)	-0.0034(5)	-0.0035(5)	-0.0091(5)
C9	0.0376(7)	0.0385(7)	0.0294(6)	-0.0048(5)	-0.0056(5)	-0.0057(5)
C10	0.0382(7)	0.0351(6)	0.0310(6)	-0.0036(5)	-0.0075(5)	-0.0066(5)
C11	0.0398(7)	0.0337(6)	0.0370(7)	-0.0048(5)	-0.0060(5)	-0.0110(5)
C12	0.0371(6)	0.0342(6)	0.0294(6)	-0.0077(5)	-0.0063(5)	-0.0051(5)
C13	0.0411(7)	0.0328(7)	0.0558(8)	-0.0126(6)	-0.0133(6)	-0.0020(6)
C14	0.0370(7)	0.0443(8)	0.0564(9)	-0.0163(6)	-0.0112(6)	-0.0048(6)
C15	0.0469(7)	0.0423(7)	0.0353(7)	-0.0118(5)	-0.0043(5)	-0.0160(6)
C16	0.0501(8)	0.0313(6)	0.0416(7)	-0.0049(5)	-0.0059(6)	-0.0072(6)
C17	0.0357(7)	0.0363(7)	0.0390(7)	-0.0039(5)	-0.0068(5)	-0.0034(5)
C18	0.0905(13)	0.0529(10)	0.0721(12)	-0.0199(8)	-0.0018(10)	-0.0361(9)
C19	0.0402(7)	0.0426(7)	0.0312(6)	-0.0054(5)	-0.0007(5)	-0.0153(6)
C20	0.0441(8)	0.0598(9)	0.0327(7)	-0.0076(6)	-0.0049(6)	-0.0128(7)
C21	0.0606(9)	0.0726(11)	0.0313(7)	-0.0119(7)	-0.0026(6)	-0.0195(8)
C22	0.0581(9)	0.0745(11)	0.0378(8)	-0.0183(7)	0.0091(7)	-0.0153(8)
C23	0.0418(8)	0.0675(10)	0.0483(8)	-0.0151(7)	0.0046(6)	-0.0117(7)
C24	0.0399(7)	0.0559(8)	0.0374(7)	-0.0100(6)	-0.0025(6)	-0.0144(6)
C25	0.0374(7)	0.0515(8)	0.0314(6)	-0.0119(6)	-0.0026(5)	-0.0100(6)
C26	0.0475(8)	0.0519(9)	0.0571(9)	-0.0063(7)	-0.0119(7)	-0.0145(7)
C27	0.0568(10)	0.0576(10)	0.0769(12)	-0.0155(8)	-0.0031(8)	-0.0217(8)
C28	0.0499(9)	0.0849(13)	0.0596(10)	-0.0312(9)	0.0028(7)	-0.0299(9)
C29	0.0494(9)	0.1078(15)	0.0464(9)	-0.0151(9)	-0.0129(7)	-0.0269(9)
C30	0.0463(8)	0.0746(11)	0.0391(8)	-0.0017(7)	-0.0096(6)	-0.0178(7)
C31	0.0801(15)	0.179(3)	0.0954(17)	-0.0430(17)	-0.0093(13)	-0.0758(17)
C32	0.0532(8)	0.0350(7)	0.0434(7)	-0.0041(6)	-0.0120(6)	-0.0134(6)
N1	0.0352(6)	0.0461(6)	0.0299(5)	-0.0082(4)	-0.0058(4)	-0.0081(5)
N2	0.0551(7)	0.0361(6)	0.0374(6)	-0.0075(5)	-0.0077(5)	-0.0100(5)
O1	0.0790(8)	0.0337(5)	0.0574(7)	-0.0105(5)	-0.0192(6)	-0.0066(5)
O2	0.0942(9)	0.0348(5)	0.0507(6)	-0.0021(4)	-0.0326(6)	-0.0002(5)
O3	0.0583(7)	0.0518(6)	0.0704(7)	-0.0157(5)	-0.0097(5)	-0.0250(5)
O4	0.0743(9)	0.1212(13)	0.0967(11)	-0.0385(9)	-0.0052(8)	-0.0553(9)
C33	0.117(6)	0.052(4)	0.078(4)	0.000(3)	-0.050(3)	0.015(4)
C34	0.182(6)	0.050(3)	0.070(3)	0.005(2)	-0.053(3)	0.014(4)
C35	0.208(6)	0.181(8)	0.088(5)	0.033(4)	-0.017(4)	-0.012(5)
C36	0.212(9)	0.075(3)	0.083(5)	0.017(3)	-0.053(5)	0.024(5)

from the surface to the nearest nucleus internal to the surface, d_e = Distance from the surface to the nearest nucleus external to the surface, Shape index = Qualitative measure of shape and Curvedness = Function of the root-mean-square curvature of the surface. The bright red spots in the sub sects' b and c of **Fig. 3**, **5**, and **7** are the hydrogen bonding centers and the weak and long range intermolecular interactions are indicated with the pale colours. In the shape index, the bright-red spot exemplifies the hydrogen bonding interactions while the blue spots indicate the complementary hydrogen bonding interactions.

Fingerprint plots are depicted in **Fig. 4**, **6** and **8**. Percentile contributions of the finger print plots are given as supplementary data (as MS Excel spreadsheet) and it can be accessed at https://data.mendeley.com/datasets/4p5t89zs4v/draft?a=b8bfd08f-a27c-4919-ae70-0648f7ed9116. In the finger prints, the colour of each point corresponds to the relative area of the surface with that (de, di) pair. Grey area is indicative of no contribution on the surface and blue colour is indicative of the relative area of the surface corresponding to each kind of interaction.

Table 3
Bond distance (Å) for compound **1.**

Bond distances (Å)			
C1-C6	1.374(2)	C19-C24	1.4017(19)
C1-C2	1.377(3)	C19-C20	1.4058(19)
C1-H1	0.93	C20-C21	1.383(2)
C2-C3	1.357(3)	C20-H20	0.93
C2-H2	0.93	C21-C22	1.379(2)
C3-C4	1.371(3)	C21-H21	0.93
C3-H3	0.93	C22-C23	1.376(2)
C4-C5	1.386(3)	C22-H22	0.93
C4-H4	0.93	C23-C24	1.379(2)
C5-C6	1.380(2)	C23-H23	0.93
C5-H5	0.93	C24-H24	0.93
C6-N2	1.4214(17)	C25-C30	1.383(2)
C7-N2	1.3529(17)	C25-C26	1.386(2)
C7-C11	1.3669(18)	C26-C27	1.381(2)
C7-C8	1.4978(18)	C26-H26	0.93
C8-C9	1.5456(17)	C27-C28	1.376(3)
C8-H8A	0.97	C27-H27	0.93
C8-H8B	0.97	C28-C29	1.373(3)
C9-N1	1.4602(15)	C28-O4	1.376(2)
C9-C25	1.5188(18)	C29-C30	1.395(2)
C9-H9	0.98	C29-H29	0.93
C10-N1	1.4678(16)	C30-H30	0.93
C10-C11	1.5159(17)	C31-O4	1.405(3)
C10-C12	1.5328(18)	C31-H31A	0.96
C10-H10	0.98	C31-H31B	0.96
C11-C32	1.4412(19)	C31-H31C	0.96
C12-C17	1.3804(18)	C32-O1	1.2232(17)
C12-C13	1.3964(18)	C32-O2	1.3465(17)
C13-C14	1.376(2)	N2-H2A	0.877(19)
C13-H13	0.93	O2-C33	1.513(18)
C14-C15	1.383(2)	C33-C34	1.490(13)
C14-H14	0.93	C33-H33A	0.97
C15-O3	1.3738(17)	C33-H33B	0.97
C15-C16	1.378(2)	C34-C35	1.481(11)
C16-C17	1.3884(19)	C34-C36	1.523(8)
C16-H16	0.93	C34-H34	0.98
C17-H17	0.93	C35-H35A	0.96
C18-O3	1.415(2)	C35-H35B	0.96
C18-H18A	0.96	C35-H35C	0.96
C18-H18B	0.96	C36-H36A	0.96
C18-H18C	0.96	C36-H36B	0.96
C19-N1	1.3925(16)	C36-H36C	0.96
H(2A) ••••O(1)	2.000(19)	N(2)-H(2A) ••••O(1)	2.6933(16)

2. Experimental Design, Materials and Methods

*2.1. Synthesis of isobutyl-1,2,6-triaryl-4-(arylamino)-1,2,5,6-tetrahydropyridine-3-carboxylates **(1-3)***

The procedure for the synthesis of **1-3** is given in the source article."The reactions were performed at room temperature under atmospheric pressure without any inert atmospheric conditions. In a 100 mL round bottomed flask, aromatic amine (1.0 mmol), isobutyl acetoacetate (0.5 mmol), sulfamic acid (catalyst; 0.1 mmol) and ethanol (75 mL) were added successively, and finally the aromatic aldehyde (1.0 mmol) was added. Initially, the reaction mixture was stirred at a slower rate and after the uniform mixing was ensured, the reaction mixture was vigorously agitated up to the completion of the reaction (7-12 hrs). The reaction was monitored by thin

Table 4
Bond angles (°) for compound **1.**

Bond angles (°)					
C6-C1-C2	120.09(17)	C13-C14-C15	120.13(13)	C28-C29-C30	119.78(15)
C6-C1-H1	120	C13-C14-H14	119.9	C28-C29-H29	120.1
C2-C1-H1	120	C15-C14-H14	119.9	C30-C29 H29	120.1
C3-C2-C1	120.49(18)	O3-C15-C16	124.07(13)	C25-C30-C29	121.34(16)
C3-C2-H2	119.8	O3-C15-C14	116.20(12)	C25-C30-H30	119.3
C1-C2-H2	119.8	C16-C15-C14	119.74(13)	C29-C30-H30	119.3
C2-C3-C4	120.26(17)	C15-C16-C17	119.44(12)	O4-C31-H31A	109.5
C2-C3-H3	119.9	C15-C16-H16	120.3	O4-C31-H31B	109.5
C4-C3-H3	119.9	C17-C16-H16	120.3	H31A-C31-H31B	109.5
C3-C4-C5	119.78(18)	C12-C17-C16	122.01(12)	O4-C31-H31C	109.5
C3-C4-H4	120.1	C12-C17-H17	119	H31A-C31-H31C	109.5
C5-C4-H4	120.1	C16-C17-H17	119	H31B-C31-H31C	109.5
C6-C5-C4	119.89(17)	O3-C18-H18A	109.5	O1-C32-O2	121.47(12)
C6-C5-H5	120.1	O3-C18-H18B	109.5	O1-C32-C11	125.80(13)
C4-C5-H5	120.1	H18A-C18-H18B	109.5	O2-C32-C11	112.73(12)
C1-C6-C5	119.47(14)	O3-C18-H18C	109.5	C19-N1-C9	119.62(10)
C1-C6-N2	119.21(13)	H18A-C18-H18C	109.5	C19-N1-C10	120.10(10)
C5-C6-N2	121.27(13)	H18B-C18-H18C	109.5	C9-N1-C10	119.18(10)
N2-C7-C11	124.31(12)	N1-C19-C24	121.31(12)	C7-N2-C6	126.84(12)
N2-C7-C8	119.92(11)	N1-C19-C20	121.62(12)	C7-N2-H2A	114.7(12)
C11-C7-C8	115.65(11)	C24-C19-C20	117.06(12)	C6-N2-H2A	118.0(12)
C7-C8-C9	109.52(10)	C21-C20-C19	120.94(14)	C32-O2-C33	118.4(5)
C7-C8-H8A	109.8	C21-C20-H20	119.5	C15-O3-C18	116.80(13)
C9-C8-H8A	109.8	C19-C20-H20	119.5	C28-O4-C31	117.84(19)
C7-C8-H8B	109.8	C22-C21-C20	121.21(14)	C34-C33-O2	104.1(12)
C9-C8-H8B	109.8	C22-C21-H21	119.4	C34-C33-H33A	110.9
H8A-C8-H8B	108.2	C20-C21-H21	119.4	O2-C33-H33A	110.9
N1-C9-C25	113.99(10)	C23-C22-C21	118.27(14)	C34-C33-H33B	110.9
N1-C9-C8	109.98(10)	C23-C22-H22	120.9	O2-C33-H33B	110.9
C25-C9-C8	109.69(10)	C21-C22-H22	120.9	H33A-C33-H33B	109
N1-C9-H9	107.6	C22-C23-C24	121.75(14)	C35-C34-C33	115.1(10)
C25-C9-H9	107.6	C22-C23-H23	119.1	C35-C34-C36	106.0(8)
C8-C9-H9	107.6	C24-C23-H23	119.1	C33-C34-C36	107.2(10)
N1-C10-C11	110.35(10)	C23-C24-C19	120.77(13)	C35-C34-H34	109.4
N1-C10-C12	112.97(10)	C23-C24-H24	119.6	C33-C34-H34	109.4
C11-C10-C12	113.22(10)	C19-C24-H24	119.6	C36-C34-H34	109.4
N1-C10-H10	106.6	C30-C25-C26	117.56(14)	C34-C35-H35A	109.5
C11-C10-H10	106.6	C30-C25-C9	119.69(13)	C34-C35-H35B	109.5
C12-C10-H10	106.6	C26-C25-C9	122.69(12)	H35A-C35-H35B	109.5
C7-C11-C32	120.97(12)	C27-C26-C25	121.44(15)	C34-C35-H35C	109.5
C7-C11-C10	117.77(11)	C27-C26-H26	119.3	H35A-C35-H35C	109.5
C32-C11-C10	121.25(11)	C25-C26-H26	119.3	H35B-C35-H35C	109.5
C17-C12-C13	117.28(12)	C28-C27-C26	120.21(17)	C34-C36-H36A	109.5
C17-C12-C10	122.32(11)	C28-C27-H27	119.9	C34-C36-H36B	109.5
C13-C12-C10	120.33(11)	C26-C27-H27	119.9	H36A-C36-H36B	109.5
C14-C13-C12	121.41(12)	C29-C28-O4	124.72(17)	C34-C36-H36C	109.5
C14-C13-H13	119.3	C29-C28-C27	119.65(15)	H36A-C36-H36C	109.5
C12-C13-H13	119.3	O4-C28-C27	115.61(18)	H36B-C36-H36C	109.5
N(2)-H(2A)••••O(1)	135.0(16)				

layer chromatography (TLC) at regular intervals. When the reaction is completed, the separated solid was filtered and washed thoroughly with aqueous ethanol. The crude products were further purified by column chromatography on silica gel (Ethyl Acetate (EtOAc)/Pet.ether, 1:9 ratio). Single crystals suitable for X-ray diffraction were obtained by the slow evaporation technique using ethanol:dichloromethane (7:3) solvent mixture".

Table 5
Torsional angles [°] for compound **1.**

Torsional angles [°]			
C6-C1-C2-C3	0.9(3)	C8-C9-C25-C30	82.97(15)
C1-C2-C3-C4	0.8(3)	N1-C9-C25-C26	29.73(18)
C2-C3-C4-C5	-1.5(3)	C8-C9-C25-C26	-94.09(15)
C3-C4-C5-C6	0.6(3)	C30-C25-C26-C27	-1.4(2)
C2-C1-C6-C5	-1.7(2)	C9-C25-C26-C27	175.71(14)
C2-C1-C6-N2	175.59(15)	C25-C26-C27-C28	-0.1(3)
C4-C5-C6-C1	1.0(2)	C26-C27-C28-C29	1.4(3)
C4-C5-C6-N2	-176.28(15)	C26-C27-C28-O4	-179.98(15)
N2-C7-C8-C9	-127.50(12)	O4-C28-C29-C30	-179.69(15)
C11-C7-C8-C9	48.80(15)	C27-C28-C29-C30	-1.2(3)
C7-C8-C9-N1	-53.98(14)	C26-C25-C30-C29	1.6(2)
C7-C8-C9-C25	72.15(13)	C9-C25-C30-C29	-175.61(14)
N2-C7-C11-C32	-2.0(2)	C28-C29-C30-C25	-0.3(3)
C8-C7-C11-C32	-178.08(12)	C7-C11-C32-O1	2.1(2)
N2-C7-C11-C10	177.19(12)	C10-C11-C32-O1	-177.05(14)
C8-C7-C11-C10	1.08(17)	C7-C11-C32-O2	-177.53(12)
N1-C10-C11-C7	-44.49(15)	C10-C11-C32-O2	3.33(19)
C12-C10-C11-C7	83.25(14)	C24-C19-N1-C9	-15.20(19)
N1-C10-C11-C32	134.67(13)	C20-C19-N1-C9	163.97(12)
C12-C10-C11-C32	-97.59(14)	C24-C19-N1-C10	176.91(12)
N1-C10-C12-C17	-0.03(17)	C20-C19-N1-C10	-3.92(19)
C11-C10-C12-C17	-126.39(13)	C25-C9-N1-C19	79.21(14)
N1-C10-C12-C13	-176.83(11)	C8-C9-N1-C19	-157.13(11)
C11-C10-C12-C13	56.80(16)	C25-C9-N1-C10	-112.79(12)
C17-C12-C13-C14	-0.3(2)	C8-C9-N1-C10	10.87(15)
C10-C12-C13-C14	176.66(12)	C11-C10-N1-C19	-155.38(11)
C12-C13-C14-C15	-0.1(2)	C12-C10-N1-C19	76.75(14)
C13-C14-C15-O3	-179.79(13)	C11-C10-N1-C9	36.68(15)
C13-C14-C15-C16	0.6(2)	C12-C10-N1-C9	-91.19(13)
O3-C15-C16-C17	179.76(12)	C11-C7-N2-C6	170.34(13)
C14-C15-C16-C17	-0.7(2)	C8-C7-N2-C6	-13.7(2)
C13-C12-C17-C16	0.24(19)	C1-C6-N2-C7	122.95(16)
C10-C12-C17-C16	-176.66(12)	C5-C6-N2-C7	-59.8(2)
C15-C16-C17-C12	0.2(2)	O1-C32-O2-C33	-7.1(8)
N1-C19-C20-C21	-179.44(14)	C11-C32-O2-C33	172.6(8)
C24-C19-C20-C21	-0.2(2)	C16-C15-O3-C18	-21.3(2)
C19-C20-C21-C22	0.0(2)	C14-C15-O3-C18	159.08(14)
C20-C21-C22-C23	-0.2(3)	C29-C28-O4-C31	-5.5(3)
C21-C22-C23-C24	0.6(3)	C27-C28-O4-C31	175.94(19)
C22-C23-C24-C19	-0.8(2)	C32-O2-C33-C34	160.3(7)
N1-C19-C24-C23	179.82(13)	O2-C33-C34-C35	-58.3(13)
C20-C19-C24-C23	0.6(2)	O2-C33-C34-C36	-175.9(10)
N1-C9-C25-C30	-153.21(13)		

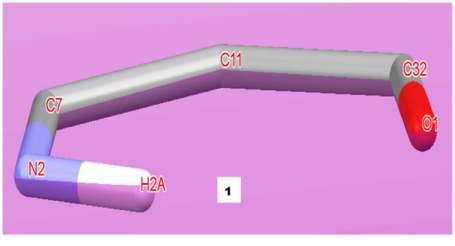
Table 6
Atomic coordinates and equivalent isotropic atomic displacement parameters (Å) for compound **2.**

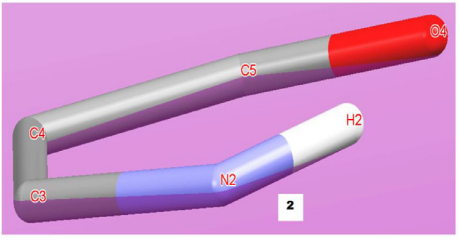
	x/a	y/b	z/c	U (eq)
F1	0.65860(14)	0.21604(13)	1.08335(10)	0.0389(4)
F2	0.54046(17)	0.94085(17)	0.09024(11)	0.0545(5)
O1	0.91637(16)	0.85354(15)	0.58988(13)	0.0330(4)
O2	-0.03237(16)	0.32345(14)	0.71665(12)	0.0290(4)
O3	0.11899(15)	0.79776(13)	0.80742(11)	0.0255(3)
O4	0.18907(16)	0.93830(14)	0.66745(12)	0.0288(4)
N1	0.45448(17)	0.54527(16)	0.74331(13)	0.0241(4)
N2	0.36618(19)	0.85201(17)	0.51325(14)	0.0251(4)
C1	0.5411(2)	0.56523(19)	0.64186(16)	0.0232(4)
C2	0.4529(2)	0.62907(19)	0.55678(16)	0.0241(4)

(*continued on next page*)

Table 6 (*continued*)

	x/a	y/b	z/c	U (eq)
C3	0.3638(2)	0.74323(19)	0.58258(16)	0.0225(4)
C4	0.2911(2)	0.72934(19)	0.68088(16)	0.0226(4)
C5	0.1986(2)	0.8314(2)	0.71535(16)	0.0241(4)
C6	0.0185(2)	0.8935(2)	0.84360(18)	0.0307(5)
C7	-0.0533(2)	0.8423(2)	0.95052(18)	0.0323(5)
C8	-0.1582(3)	0.9456(3)	0.9884(2)	0.0460(7)
C9	-0.1177(3)	0.7413(3)	0.9534(2)	0.0573(9)
C10	0.3100(2)	0.60340(19)	0.75265(16)	0.0223(4)
C11	0.2238(2)	0.52575(19)	0.73899(16)	0.0227(4)
C12	0.0858(2)	0.57350(19)	0.73648(17)	0.0258(4)
C13	0.0032(2)	0.50388(19)	0.73017(17)	0.0268(5)
C14	0.0575(2)	0.38449(19)	0.72480(16)	0.0245(4)
C15	0.1934(2)	0.3351(2)	0.72629(17)	0.0266(5)
C16	0.2750(2)	0.40632(19)	0.73358(17)	0.0262(5)
C17	0.0050(3)	0.1952(2)	0.74688(19)	0.0335(5)
C18	0.5057(2)	0.46183(19)	0.82859(16)	0.0240(4)
C19	0.4200(2)	0.4211(2)	0.92133(16)	0.0264(5)
C20	0.4714(2)	0.3394(2)	1.00634(17)	0.0293(5)
C21	0.6086(2)	0.2966(2)	0.99904(17)	0.0291(5)
C22	0.6958(2)	0.3324(2)	0.91019(18)	0.0289(5)
C23	0.6449(2)	0.4145(2)	0.82468(17)	0.0260(5)
C24	0.6431(2)	0.63967(19)	0.63083(16)	0.0231(4)
C25	0.7550(2)	0.6342(2)	0.55142(17)	0.0272(5)
C26	0.8475(2)	0.7048(2)	0.53391(18)	0.0303(5)
C27	0.8295(2)	0.7820(2)	0.59755(17)	0.0257(5)
C28	0.7190(2)	0.7878(2)	0.67746(18)	0.0277(5)
C29	0.6264(2)	0.71774(19)	0.69350(17)	0.0252(4)
C30	1.0326(2)	0.8465(2)	0.51033(19)	0.0359(6)
C31	0.4154(2)	0.86947(19)	0.40466(16)	0.0240(4)
C32	0.5076(2)	0.9417(2)	0.35809(18)	0.0287(5)
C33	0.5505(2)	0.9667(2)	0.25166(19)	0.0340(5)
C34	0.4998(2)	0.9168(2)	0.19434(17)	0.0354(6)
C35	0.4105(2)	0.8435(2)	0.23796(18)	0.0338(5)
C36	0.3663(2)	0.8204(2)	0.34432(17)	0.0293(5)





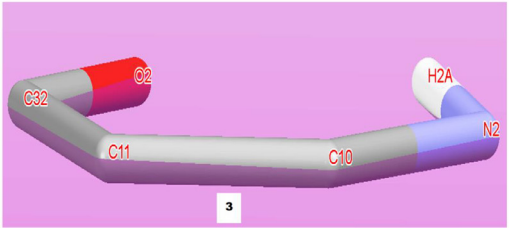


Fig. 2. Plane of pseudo six membered ring (RAHB) in **1, 2** and **3**.

Table 7
Anisotropic atomic displacement parameters (Å) for compound **2.**

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F1	0.0428(8)	0.0428(8)	0.0283(7)	0.0050(6)	-0.0170(6)	-0.0108(7)
F2	0.0513(10)	0.0811(13)	0.0190(7)	-0.0019(7)	0.0002(6)	-0.0125(9)
O1	0.0303(9)	0.0381(9)	0.0342(9)	-0.0083(7)	-0.0036(7)	-0.0156(7)
O2	0.0310(8)	0.0240(8)	0.0360(9)	-0.0101(6)	-0.0061(7)	-0.0092(7)
O3	0.0269(8)	0.0272(8)	0.0226(8)	-0.0095(6)	-0.0005(6)	-0.0062(6)
O4	0.0361(9)	0.0236(8)	0.0277(8)	-0.0071(6)	-0.0031(7)	-0.0095(7)
N1	0.0209(9)	0.0283(10)	0.0202(9)	-0.0031(7)	-0.0036(7)	-0.0042(7)
N2	0.0301(10)	0.0246(10)	0.0210(9)	-0.0064(7)	-0.0026(7)	-0.0077(8)
C1	0.0244(10)	0.0255(11)	0.0192(10)	-0.0035(8)	-0.0052(8)	-0.0057(8)
C2	0.0265(11)	0.0260(11)	0.0204(10)	-0.0066(8)	-0.0052(8)	-0.0047(9)
C3	0.0225(10)	0.0276(11)	0.0206(10)	-0.0073(8)	-0.0067(8)	-0.0064(8)
C4	0.0252(10)	0.0237(10)	0.0205(10)	-0.0070(8)	-0.0044(8)	-0.0059(8)
C5	0.0278(11)	0.0285(11)	0.0199(10)	-0.0074(8)	-0.0036(8)	-0.0113(9)
C6	0.0324(12)	0.0309(12)	0.0270(12)	-0.0113(9)	-0.0024(9)	-0.0024(10)
C7	0.0321(12)	0.0414(14)	0.0250(12)	-0.0115(10)	-0.0036(9)	-0.0080(10)
C8	0.0356(14)	0.0613(18)	0.0338(14)	-0.0173(13)	-0.0013(11)	0.0025(13)
C9	0.069(2)	0.073(2)	0.0418(17)	-0.0225(15)	0.0145(15)	-0.0463(18)
C10	0.0219(10)	0.0244(10)	0.0209(10)	-0.0063(8)	-0.0028(8)	-0.0058(8)
C11	0.0252(10)	0.0236(10)	0.0196(10)	-0.0046(8)	-0.0043(8)	-0.0062(8)
C12	0.0243(11)	0.0215(10)	0.0310(12)	-0.0072(8)	-0.0044(9)	-0.0035(8)
C13	0.0246(11)	0.0239(11)	0.0323(12)	-0.0059(9)	-0.0062(9)	-0.0059(9)
C14	0.0296(11)	0.0229(10)	0.0223(11)	-0.0052(8)	-0.0048(8)	-0.0085(9)
C15	0.0305(11)	0.0233(11)	0.0263(11)	-0.0092(8)	-0.0056(9)	-0.0029(9)
C16	0.0264(11)	0.0261(11)	0.0257(11)	-0.0076(9)	-0.0084(9)	-0.0006(9)
C17	0.0469(14)	0.0255(12)	0.0327(13)	-0.0066(9)	-0.0105(11)	-0.0128(11)
C18	0.0270(11)	0.0253(11)	0.0201(10)	-0.0035(8)	-0.0063(8)	-0.0071(9)
C19	0.0252(11)	0.0316(12)	0.0230(11)	-0.0045(9)	-0.0057(8)	-0.0088(9)
C20	0.0341(12)	0.0341(12)	0.0204(11)	-0.0015(9)	-0.0059(9)	-0.0133(10)
C21	0.0368(13)	0.0286(11)	0.0233(11)	0.0002(9)	-0.0137(9)	-0.0097(10)
C22	0.0269(11)	0.0314(12)	0.0286(12)	-0.0052(9)	-0.0105(9)	-0.0044(9)
C23	0.0265(11)	0.0278(11)	0.0237(11)	-0.0040(8)	-0.0070(8)	-0.0066(9)
C24	0.0231(10)	0.0274(11)	0.0188(10)	-0.0046(8)	-0.0047(8)	-0.0059(9)
C25	0.0273(11)	0.0337(12)	0.0225(11)	-0.0088(9)	-0.0028(8)	-0.0089(9)
C26	0.0287(12)	0.0375(13)	0.0247(11)	-0.0075(9)	-0.0011(9)	-0.0108(10)
C27	0.0250(11)	0.0270(11)	0.0259(11)	-0.0029(8)	-0.0081(8)	-0.0076(9)
C28	0.0285(11)	0.0272(11)	0.0289(12)	-0.0088(9)	-0.0069(9)	-0.0050(9)
C29	0.0240(11)	0.0274(11)	0.0228(11)	-0.0062(8)	-0.0048(8)	-0.0031(9)
C30	0.0316(13)	0.0475(15)	0.0324(13)	-0.0068(11)	-0.0055(10)	-0.0183(11)
C31	0.0249(11)	0.0238(10)	0.0201(10)	-0.0047(8)	-0.0023(8)	-0.0027(8)
C32	0.0301(12)	0.0255(11)	0.0305(12)	-0.0067(9)	-0.0037(9)	-0.0077(9)
C33	0.0343(13)	0.0296(12)	0.0294(13)	0.0004(9)	0.0013(10)	-0.0076(10)
C34	0.0355(13)	0.0427(14)	0.0180(11)	-0.0003(10)	-0.0030(9)	-0.0020(11)
C35	0.0342(13)	0.0434(14)	0.0231(12)	-0.0084(10)	-0.0075(9)	-0.0054(11)
C36	0.0301(12)	0.0337(12)	0.0254(11)	-0.0061(9)	-0.0061(9)	-0.0096(10)

Table 8
Bond distances (Å) for compound **2.**

Bond distances (Å)					
F1-C21	1.365(2)	C7-C8	1.525(4)	C20-H20	0.95
F2-C34	1.349(3)	C7-H7	1.00	C21-C22	1.365(3)
O1-C27	1.373(3)	C8-H8A	0.98	C22-C23	1.387(3)
O1-C30	1.424(3)	C8-H8B	0.98	C22-H22	0.95
O2-C14	1.377(2)	C8-H8C	0.98	C23-H23	0.95
O2-C17	1.417(3)	C9-H9A	0.98	C24-C29	1.390(3)
O3-C5	1.348(3)	C9-H9B	0.98	C24-C25	1.393(3)
O3-C6	1.434(3)	C9-H9C	0.98	C25-C26	1.384(3)
O4-C5	1.229(3)	C10-C11	1.531(3)	C25-H25	0.95

(*continued on next page*)

Table 8 (*continued*)

Bond distances (Å)					
N1-C18	1.392(3)	C10-H10	1.00	C26-C27	1.390(3)
N1-C1	1.456(3)	C11-C16	1.384(3)	C26-H26	0.95
N1-C10	1.466(3)	C11-C12	1.399(3)	C27-C28	1.388(3)
N2-C3	1.356(3)	C12-C13	1.383(3)	C28-C29	1.384(3)
N2-C31	1.420(3)	C12-H12	0.95	C28-H28	0.95
N2-H2	0.89(3)	C13-C14	1.387(3)	C29-H29	0.95
C1-C24	1.519(3)	C13-H13	0.95	C30-H30A	0.98
C1-C2	1.540(3)	C14-C15	1.379(3)	C30-H30B	0.98
C1-H1	1.00	C15-C16	1.394(3)	C30-H30C	0.98
C2-C3	1.499(3)	C15-H15	0.95	C31-C32	1.382(3)
C2-H2A	0.99	C16-H16	0.95	C31-C36	1.392(3)
C2-H2AB	0.99	C17-H17A	0.98	C32-C33	1.381(3)
C3-C4	1.362(3)	C17-H17B	0.98	C32-H32	0.95
C4-C5	1.445(3)	C17-H17C	0.98	C33-C34	1.377(4)
C4-C10	1.511(3)	C18-C23	1.399(3)	C33-H33	0.95
C6-C7	1.505(3)	C18-C19	1.404(3)	C34-C35	1.363(4)
C6-H6A	0.99	C19-C20	1.383(3)	C35-C36	1.382(3)
C6-H6AB	0.99	C19-H19	0.95	C35-H35	0.95
C7-C9	1.515(4)	C20-C21	1.370(3)	C36-H36	0.95
H(2) ••••O(4)	1.986(3)	N(2)-H(2) ••••O(4)	2.696(3)		

Table 9
Bond angles (°) for compound **2.**

Bond angles (°)					
C27-O1-C30	116.52(18)	C7-C9-H9A	109.5	C21-C22-C23	119.4(2)
C14-O2-C17	116.38(17)	C7-C9-H9B	109.5	C21-C22-C22	120.3
C5-O3-C6	116.02(17)	H9A-C9-H9B	109.5	C23-C22-H22	120.3
C18-N1-C1	119.95(17)	C7-C9-H9C	109.5	C22-C23-C18	121.0(2)
C18-N1-C10	120.12(17)	H9A-C9-H9C	109.5	C22-C23-H23	119.5
C1-N1-C10	119.60(16)	H9B-C9-H9C	109.5	C18-C23-H23	119.5
C3-N2-C31	125.41(19)	N1-C10-C4	109.45(17)	C29-C24-C25	118.3(2)
C3-N2-H2	114.0(18)	N1-C10-C11	113.21(17)	C29-C24-C1	122.81(19)
C31-N2-H2	119.3(18)	C4-C10-C11	113.77(17)	C25-C24-C1	118.80(19)
N1-C1-C24	114.43(17)	N1-C10-H10	106.6	C26-C25-C24	121.5(2)
N1-C1-C2	109.36(17)	C4-C10-H10	106.6	C26-C25-H25	119.3
C24-C1-C2	108.60(17)	C11-C10-H10	106.6	C24-C25-H25	119.3
N1-C1-H1	108.1	C16-C11-C12	117.4(2)	C25-C26-C27	119.4(2)
C24-C1-H1	108.1	C16-C11-C10	122.74(19)	C25-C26-H26	120.3
C2-C1-H1	108.1	C12-C11-C10	119.78(18)	C27-C26-H26	120.3
C3-C2-C1	108.16(17)	C13-C12-C11	121.4(2)	O1-C27-C28	115.5(2)
C3-C2-H2A	110.1	C13-C12-H12	119.3	O1-C27-C26	124.8(2)
C1-C2-H2A	110.1	C11-C12-H12	119.3	C28-C27-C26	119.7(2)
C3-C2-H2AB	110.1	C12-C13-C14	119.8(2)	C29-C28-C27	120.3(2)
C1-C2-H2AB	110.1	C12-C13-H13	120.1	C29-C28-H28	119.8
H2A-C2-H2AB	108.4	C14-C13-H13	120.1	C27-C28-H28	119.8
N2-C3-C4	124.0(2)	O2-C14-C15	124.41(19)	C28-C29-C24	120.7(2)
N2-C3-C2	120.41(19)	O2-C14-C13	115.45(19)	C28-C29-H29	119.6
C4-C3-C2	115.37(18)	C15-C14-C13	120.1(2)	C24-C29-H29	119.6
C3-C4-C5	121.21(19)	C14-C15-C16	119.3(2)	O1-C30-H30A	109.5
C3-C4-C10	117.74(19)	C14-C15-H15	120.4	O1-C30-H30B	109.5
C5-C4-C10	121.05(18)	C16-C15-H15	120.4	H30A-C30-H30B	109.5
O4-C5-O3	121.9(2)	C11-C16-C15	121.9(2)	O1-C30-H30C	109.5
O4-C5-C4	125.4(2)	C11-C16-H16	119	H30A-C30-H30C	109.5
O3-C5-C4	112.76(18)	C15-C16-H16	119	H30B-C30-H30C	109.5
O3-C6-C7	109.18(19)	O2-C17-H17A	109.5	C32-C31-C36	120.0(2)
O3-C6-H6A	109.8	O2-C17-H17B	109.5	C32-C31-N2	119.13(19)
C7-C6-H6A	109.8	H17A-C17-H17B	109.5	C36-C31-N2	120.8(2)
O3-C6-H6AB	109.8	O2-C17-H17C	109.5	C33-C32-C31	120.5(2)

(*continued on next page*)

Table 9 (*continued*)

Bond angles (°)					
C7-C6-H6AB	109.8	H17A-C17-H17C	109.5	C33-C32-H32	119.8
H6A-C6-H6AB	108.3	H17B-C17-H17C	109.5	C31-C32-H32	119.8
C6-C7-C9	112.8(2)	N1-C18-C23	121.07(19)	C34-C33-C32	118.0(2)
C6-C7-C8	108.5(2)	N1-C18-C19	121.43(19)	C34-C33-H33	121
C9-C7-C8	111.2(2)	C23-C18-C19	117.50(19)	C32-C33-H33	121
C6-C7-H7	108.1	C20-C19-C18	121.3(2)	F2-C34-C35	118.3(2)
C9-C7-H7	108.1	C20-C19-H19	119.4	F2-C34-C33	118.7(2)
C8-C7-H7	108.1	C18-C19-H19	119.4	C35-C34-C33	123.0(2)
C7-C8-H8A	109.5	C21-C20-C19	119.1(2)	C34-C35-C36	118.6(2)
C7-C8-H8B	109.5	C21-C20-H20	120.5	C34-C35-H35	120.7
H8A-C8-H8B	109.5	C19-C20-H20	120.5	C36-C35-H35	120.7
C7-C8-H8C	109.5	F1-C21-C22	119.4(2)	C35-C36-C31	119.9(2)
H8A-C8-H8C	109.5	F1-C21-C20	118.7(2)	C35-C36-H36	120
H8B-C8-H8C	109.5	C22-C21-C20	121.8(2)	C31-C36-H36	120
N(2)-H(2)••••O(1)	135.99(2)				

Table 10
Torsional angles [°] for compound **2.**

Torsional angles [°]					
C30-O1-C27-C26	-0.0(3)	C3-C4-C10-N1	44.0(3)	N1-C18-C23-H23	-0.7
C30-O1-C27-C28	178.3(2)	C3-C4-C10-H10	159	C19-C18-C23-C22	-1.3(3)
C27-O1-C30-H30A	62.6	C3-C4-C10-C11	-83.7(2)	C19-C18-C23-H23	178.7
C27-O1-C30-H30B	-57.4	C5-C4-C10-N1	-136.2(2)	C18-C19-C20-H20	179.3
C27-O1-C30-H30C	-177.4	C5-C4-C10-H10	-21.3	C18-C19-C20-C21	-0.8(3)
C17-O2-C14-C13	-158.8(2)	C5-C4-C10-C11	96.0(2)	H19-C19-C20-H20	-0.6
C17-O2-C14-C15	22.2(3)	O3-C6-C7-H7	62.2	H19-C19-C20-C21	179.3
C14-O2-C17-H17A	171.2	O3-C6-C7-C8	179.1(2)	C19-C20-C21-F1	179.9(2)
C14-O2-C17-H17B	51.3	O3-C6-C7-C9	-57.2(3)	C19-C20-C21-C22	-0.0(3)
C14-O2-C17-H17C	-68.8	H6A-C6-C7-H7	-177.3	H20-C20-C21-F1	-0.1
C6-O3-C5-O4	2.8(3)	H6A-C6-C7-C8	-60.3	H20-C20-C21-C22	179.9
C6-O3-C5-C4	-176.2(2)	H6A-C6-C7-C9	63.3	F1-C21-C22-H22	0.1
C5-O3-C6-H6A	64.1	H6AB-C6-C7-H7	-58.3	F1-C21-C22-C23	-179.8(2)
C5-O3-C6-H6AB	-54.9	H6AB-C6-C7-C8	58.6	C20-C21-C22-H22	-180
C5-O3-C6-C7	-175.4(2)	H6AB-C6-C7-C9	-177.7	C20-C21-C22-C23	0.1(4)
C10-N1-C1-H1	-128.2	C6-C7-C8-H8A	-56	C21-C22-C23-C18	0.6(3)
C10-N1-C1-C2	-10.7(3)	C6-C7-C8-H8B	-176	C21-C22-C23-H23	-179.4
C10-N1-C1-C24	111.4(2)	C6-C7-C8-H8C	64	H22-C22-C23-C18	-179.3
C18-N1-C1-H1	45.2	H7-C7-C8-H8A	61	H22-C22-C23-H23	0.7
C18-N1-C1-C2	162.7(2)	H7-C7-C8-H8B	-59.1	C1-C24-C25-H25	-3.5
C18-N1-C1-C24	-75.2(2)	H7-C7-C8-H8C	-179	C1-C24-C25-C26	176.5(2)
C1-N1-C10-C4	-37.8(3)	C9-C7-C8-H8A	179.4	C29-C24-C25-H25	179.5
C1-N1-C10-H10	-152.8	C9-C7-C8-H8B	59.4	C29-C24-C25-C26	-0.5(3)
C1-N1-C10-C11	90.3(2)	C9-C7-C8-H8C	-60.5	C1-C24-C29-C28	-177.1(2)
C18-N1-C10-C4	148.8(2)	C6-C7-C9-H9A	-58.3	C1-C24-C29-H29	2.9
C18-N1-C10-H10	33.8	C6-C7-C9-H9B	-178.3	C25-C24-C29-C28	-0.2(3)
C18-N1-C10-C11	-83.1(2)	C6-C7-C9-H9C	61.8	C25-C24-C29-H29	179.8
C1-N1-C18-C19	-166.2(2)	H7-C7-C9-H9A	-177.7	C24-C25-C26-H26	-179.3
C1-N1-C18-C23	13.2(3)	H7-C7-C9-H9B	62.3	C24-C25-C26-C27	0.7(3)
C10-N1-C18-C19	7.1(3)	H7-C7-C9-H9C	-57.6	H25-C25-C26-H26	0.7
C10-N1-C18-C23	-173.5(2)	C8-C7-C9-H9A	63.8	H25-C25-C26-C27	-179.3
H2-N2-C3-C2	-174(2)	C8-C7-C9-H9B	-56.2	C25-C26-C27-O1	177.9(2)
H2-N2-C3-C4	1(2)	C8-C7-C9-H9C	-176.1	C25-C26-C27-C28	-0.3(3)
C31-N2-C3-C2	19.7(3)	N1-C10-C11-C12	-174.3(2)	H26-C26-C27-O1	-2.1
C31-N2-C3-C4	-165.4(2)	N1-C10-C11-C16	8.8(3)	H26-C26-C27-C28	179.7
H2-N2-C31-C32	65(2)	C4-C10-C11-C12	-48.5(3)	O1-C27-C28-H28	1.2
H2-N2-C31-C36	-112(2)	C4-C10-C11-C16	134.6(2)	O1-C27-C28-C29	-178.8(2)
C3-N2-C31-C32	-129.4(2)	H10-C10-C11-C12	68.8	C26-C27-C28-H28	179.5

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Table 10 (*continued*)

Torsional angles [°]					
C3-N2-C31-C36	54.2(3)	H10-C10-C11-C16	-108.1	C26-C27-C28-C29	-0.4(3)
N1-C1-C2-H2A	175.9	C10-C11-C12-H12	3.7	C27-C28-C29-C24	0.7(3)
N1-C1-C2-H2AB	-64.7	C10-C11-C12-C13	-176.3(2)	C27-C28-C29-H29	-179.3
N1-C1-C2-C3	55.6(2)	C16-C11-C12-H12	-179.2	H28-C28-C29-C24	-179.3
H1-C1-C2-H2A	-66.6	C16-C11-C12-C13	0.8(3)	H28-C28-C29-H29	0.7
H1-C1-C2-H2AB	52.8	C10-C11-C16-C15	176.8(2)	N2-C31-C32-H32	4.2
H1-C1-C2-C3	173.1	C10-C11-C16-H16	-3.2	N2-C31-C32-C33	-175.8(2)
C24-C1-C2-H2A	50.4	C12-C11-C16-C15	-0.2(3)	C36-C31-C32-H32	-179.3
C24-C1-C2-H2AB	169.8	C12-C11-C16-H16	179.8	C36-C31-C32-C33	0.7(3)
C24-C1-C2-C3	-69.9(2)	C11-C12-C13-H13	179.1	N2-C31-C36-C35	176.8(2)
N1-C1-C24-C25	161.1(2)	C11-C12-C13-C14	-0.9(3)	N2-C31-C36-H36	-3.2
N1-C1-C24-C29	-22.1(3)	H12-C12-C13-H13	-0.9	C32-C31-C36-C35	0.4(3)
H1-C1-C24-C25	40.6	H12-C12-C13-C14	179.1	C32-C31-C36-H36	-179.6
H1-C1-C24-C29	-142.6	C12-C13-C14-O2	-178.8(2)	C31-C32-C33-H33	179.4
C2-C1-C24-C25	-76.4(2)	C12-C13-C14-C15	0.3(3)	C31-C32-C33-C34	-0.6(3)
C2-C1-C24-C29	100.4(2)	H13-C13-C14-O2	1.2	H32-C32-C33-H33	-0.6
C1-C2-C3-N2	123.2(2)	H13-C13-C14-C15	-179.7	H32-C32-C33-C34	179.4
C1-C2-C3-C4	-52.1(2)	O2-C14-C15-H15	-0.8	C32-C33-C34-F2	179.8(2)
H2A-C2-C3-N2	3	O2-C14-C15-C16	179.2(2)	C32-C33-C34-C35	-0.5(4)
H2A-C2-C3-C4	-172.4	C13-C14-C15-H15	-179.8	H33-C33-C34-F2	-0.3
H2AB-C2-C3-N2	-116.5	C13-C14-C15-C16	0.2(3)	H33-C33-C34-C35	179.4
H2AB-C2-C3-C4	68.2	C14-C15-C16-C11	-0.3(3)	F2-C34-C35-H35	1.3
N2-C3-C4-C5	6.4(3)	C14-C15-C16-H16	179.7	F2-C34-C35-C36	-178.7(2)
N2-C3-C4-C10	-173.8(2)	H15-C15-C16-C11	179.7	C33-C34-C35-H35	-178.5
C2-C3-C4-C5	-178.5(2)	H15-C15-C16-H16	-0.3	C33-C34-C35-C36	1.6(4)
C2-C3-C4-C10	1.3(3)	N1-C18-C19-H19	0.7	C34-C35-C36-C31	-1.4(3)
C3-C4-C5-O3	169.2(2)	N1-C18-C19-C20	-179.1(2)	C34-C35-C36-H36	178.6
C3-C4-C5-O4	-9.8(4)	C23-C18-C19-H19	-178.7	H35-C35-C36-C31	178.6
C10-C4-C5-O3	-10.6(3)	C23-C18-C19-C20	1.4(3)	H35-C35-C36-H36	-1.4
C10-C4-C5-O4	170.5(2)	N1-C18-C23-C22	179.3(2)		

Table 11
Atomic coordinates and equivalent isotropic atomic displacement parameters (Å) for compound **3.**

	x/a	y/b	z/c	U (eq)
C1	0.2868(4)	0.6370(4)	0.6679(3)	0.0875(10)
C2	0.2375(4)	0.5099(3)	0.6300(3)	0.0871(9)
C3	0.2932(3)	0.4491(3)	0.6825(2)	0.0731(8)
C4	0.4019(3)	0.5143(2)	0.77396(19)	0.0580(6)
C5	0.4507(4)	0.6410(3)	0.8127(2)	0.0763(8)
C6	0.3926(4)	0.7008(3)	0.7609(3)	0.0922(10)
C7	0.2263(6)	0.7029(5)	0.6090(4)	0.1317(17)
C8	0.4730(3)	0.4509(2)	0.83023(18)	0.0549(6)
C9	0.6107(3)	0.4439(2)	0.80342(19)	0.0602(7)
C10	0.5728(3)	0.3593(2)	0.69196(19)	0.0555(6)
C11	0.4706(3)	0.2480(2)	0.66044(18)	0.0537(6)
C12	0.4104(3)	0.2199(2)	0.74122(17)	0.0523(6)
C13	0.4989(3)	0.1663(2)	0.79844(18)	0.0541(6)
C14	0.5192(3)	0.0574(2)	0.7432(2)	0.0714(8)
C15	0.5970(4)	0.0056(3)	0.7924(3)	0.0813(9)
C16	0.6566(3)	0.0585(3)	0.8980(3)	0.0755(8)
C17	0.6354(3)	0.1666(3)	0.9529(2)	0.0780(8)
C18	0.5585(3)	0.2200(2)	0.9042(2)	0.0667(7)
C19	0.7388(4)	-0.0009(4)	0.9520(3)	0.1093(12)
C20	0.2806(2)	0.3154(2)	0.85956(17)	0.0542(6)
C21	0.2140(3)	0.2025(3)	0.8611(2)	0.0663(7)
C22	0.1125(3)	0.1929(3)	0.9125(2)	0.0814(9)
C23	0.0770(3)	0.2940(4)	0.9608(2)	0.0846(10)
C24	0.1382(3)	0.4050(3)	0.9605(2)	0.0764(9)

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Table 11 (*continued*)

	x/a	y/b	z/c	U (eq)
C25	0.2397(3)	0.4159(2)	0.90977(18)	0.0617(7)
C26	0.7257(3)	0.5207(2)	0.6576(2)	0.0631(7)
C27	0.8640(3)	0.5607(3)	0.7166(3)	0.0961(11)
C28	0.9526(4)	0.6796(4)	0.7447(3)	0.1082(12)
C29	0.9009(5)	0.7533(3)	0.7116(3)	0.0973(11)
C30	0.7655(5)	0.7182(3)	0.6539(3)	0.1064(12)
C31	0.6762(4)	0.6002(3)	0.6268(3)	0.0878(9)
C32	0.4138(3)	0.1644(2)	0.5523(2)	0.0598(6)
C33	0.2409(4)	-0.0255(3)	0.4257(2)	0.0880(10)
C34	0.1640(4)	-0.1468(3)	0.4201(3)	0.0925(11)
C35	0.0531(5)	-0.1448(4)	0.4758(4)	0.1184(14)
C36	0.1070(5)	-0.2385(3)	0.3066(3)	0.1292(17)
N1	0.3846(2)	0.32806(17)	0.81028(15)	0.0544(5)
N2	0.6333(3)	0.3987(2)	0.6288(2)	0.0681(6)
O1	0.3068(2)	0.06252(17)	0.53247(13)	0.0757(6)
O2	0.4561(2)	0.18069(18)	0.48289(14)	0.0796(6)
F2	0.9889(3)	0.8703(2)	0.7395(2)	0.1537(11)
F1	-0.0228(2)	0.2842(2)	1.01174(18)	0.1325(9)

Table 12
Anisotropic atomic displacement parameters (Å) for compound **3.**

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.109(3)	0.101(3)	0.102(3)	0.067(2)	0.059(2)	0.059(2)
C2	0.087(2)	0.101(3)	0.077(2)	0.0401(19)	0.0169(17)	0.0400(19)
C3	0.0764(19)	0.0638(17)	0.0681(18)	0.0214(14)	0.0105(15)	0.0226(15)
C4	0.0629(16)	0.0518(14)	0.0558(15)	0.0186(12)	0.0235(13)	0.0150(12)
C5	0.091(2)	0.0578(16)	0.0743(19)	0.0250(15)	0.0295(16)	0.0161(15)
C6	0.120(3)	0.0682(19)	0.108(3)	0.047(2)	0.054(2)	0.033(2)
C7	0.171(4)	0.170(4)	0.151(4)	0.121(4)	0.089(3)	0.109(4)
C8	0.0545(14)	0.0493(13)	0.0450(13)	0.0086(10)	0.0132(11)	0.0085(11)
C9	0.0526(14)	0.0564(14)	0.0571(15)	0.0163(12)	0.0137(12)	0.0072(11)
C10	0.0502(14)	0.0593(15)	0.0544(14)	0.0211(12)	0.0175(11)	0.0166(12)
C11	0.0549(14)	0.0534(14)	0.0482(13)	0.0178(11)	0.0161(11)	0.0147(11)
C12	0.0504(13)	0.0470(13)	0.0479(13)	0.0140(10)	0.0126(11)	0.0071(10)
C13	0.0556(14)	0.0460(13)	0.0528(14)	0.0162(11)	0.0178(11)	0.0094(11)
C14	0.100(2)	0.0561(15)	0.0601(16)	0.0235(13)	0.0300(15)	0.0264(15)
C15	0.111(3)	0.0610(17)	0.089(2)	0.0367(17)	0.046(2)	0.0373(17)
C16	0.0724(19)	0.0712(18)	0.095(2)	0.0469(18)	0.0266(17)	0.0256(15)
C17	0.0723(19)	0.082(2)	0.0664(18)	0.0258(16)	0.0054(15)	0.0227(16)
C18	0.0667(17)	0.0616(16)	0.0585(16)	0.0129(13)	0.0122(13)	0.0225(13)
C19	0.113(3)	0.100(3)	0.133(3)	0.067(2)	0.026(2)	0.047(2)
C20	0.0472(13)	0.0605(15)	0.0452(13)	0.0171(11)	0.0091(11)	0.0128(11)
C21	0.0597(16)	0.0725(17)	0.0686(17)	0.0320(14)	0.0232(13)	0.0185(14)
C22	0.0672(18)	0.096(2)	0.081(2)	0.0443(18)	0.0277(16)	0.0131(17)
C23	0.0577(17)	0.115(3)	0.0670(19)	0.0260(18)	0.0292(15)	0.0167(18)
C24	0.0525(16)	0.091(2)	0.0591(17)	0.0070(15)	0.0144(13)	0.0186(15)
C25	0.0495(14)	0.0665(16)	0.0507(14)	0.0114(12)	0.0090(12)	0.0131(12)
C26	0.0670(17)	0.0620(16)	0.0633(16)	0.0277(13)	0.0286(14)	0.0174(13)
C27	0.068(2)	0.090(2)	0.139(3)	0.067(2)	0.023(2)	0.0163(17)
C28	0.071(2)	0.100(3)	0.137(3)	0.057(3)	0.023(2)	-0.002(2)
C29	0.118(3)	0.067(2)	0.100(3)	0.0367(19)	0.044(2)	0.009(2)
C30	0.147(4)	0.071(2)	0.106(3)	0.045(2)	0.031(3)	0.037(2)
C31	0.096(2)	0.077(2)	0.080(2)	0.0298(17)	0.0124(18)	0.0275(18)
C32	0.0622(16)	0.0578(15)	0.0542(15)	0.0203(12)	0.0169(13)	0.0160(13)
C33	0.105(2)	0.0731(19)	0.0500(16)	0.0070(14)	0.0095(16)	0.0073(17)
C34	0.085(2)	0.0656(19)	0.085(2)	0.0077(16)	-0.0147(18)	0.0216(17)
C35	0.104(3)	0.091(3)	0.136(4)	0.045(3)	0.017(3)	0.010(2)
C36	0.127(3)	0.081(2)	0.105(3)	-0.012(2)	-0.027(2)	0.031(2)

(*continued on next page*)

Table 12 (*continued*)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0555(12)	0.0481(11)	0.0553(12)	0.0167(9)	0.0218(10)	0.0135(9)
N2	0.0716(15)	0.0654(14)	0.0585(14)	0.0227(12)	0.0254(12)	0.0079(12)
O1	0.0836(13)	0.0643(11)	0.0472(10)	0.0078(8)	0.0136(9)	-0.0013(10)
O2	0.1001(15)	0.0756(13)	0.0514(11)	0.0207(9)	0.0267(11)	0.0152(11)
F2	0.187(3)	0.0768(14)	0.165(2)	0.0451(15)	0.061(2)	-0.0090(15)
F1	0.0960(15)	0.168(2)	0.1248(17)	0.0462(16)	0.0723(14)	0.0232(14)

Table 13
Bond distances (Å) for compound **3.**

Bond distances (Å)					
C1-C6	1.379(5)	C13-C18	1.378(3)	C26-C27	1.372(4)
C1-C2	1.381(5)	C13-C14	1.381(4)	C26-N2	1.429(3)
C1-C7	1.518(5)	C14-C15	1.379(4)	C27-C28	1.388(5)
C2-C3	1.383(4)	C14-H14	0.93	C27-H27	0.93
C2-H2	0.93	C15-C16	1.377(4)	C28-C29	1.333(5)
C3-C4	1.379(4)	C15-H15	0.93	C28-H28	0.93
C3-H3	0.93	C16-C17	1.377(4)	C29-C30	1.349(6)
C4-C5	1.377(4)	C16-C19	1.519(4)	C29-F2	1.368(4)
C4-C8	1.518(4)	C17-C18	1.384(4)	C30-C31	1.385(5)
C5-C6	1.376(4)	C17-H17	0.93	C30-H30	0.93
C5-H5	0.93	C18-H18	0.93	C31-H31	0.93
C6-H6	0.93	C19-H19A	0.96	C32-O2	1.226(3)
C7-H7A	0.96	C19-H19B	0.96	C32-O1	1.347(3)
C7-H7B	0.96	C19-H19C	0.96	C33-O1	1.447(3)
C7-H7C	0.96	C20-N1	1.392(3)	C33-C34	1.475(5)
C8-N1	1.456(3)	C20-C25	1.396(4)	C33-H33A	0.97
C8-C9	1.536(3)	C20-C21	1.401(4)	C33-H33B	0.97
C8-H8	0.98	C21-C22	1.387(4)	C34-C35	1.505(5)
C9-C10	1.491(3)	C21-H21	0.93	C34-C36	1.527(5)
C9-H9A	0.97	C22-C23	1.362(5)	C34-H34	0.98
C9-H9B	0.97	C22-H22	0.93	C35-H35A	0.96
C10-N2	1.356(3)	C23-C24	1.361(5)	C35-H35B	0.96
C10-C11	1.365(3)	C23-F1	1.370(3)	C35-H35C	0.96
C11-C32	1.443(3)	C24-C25	1.382(4)	C36-H36A	0.96
C11-C12	1.524(3)	C24-H24	0.93	C36-H36B	0.96
C12-N1	1.468(3)	C25-H25	0.93	C36-H36C	0.96
C12-C13	1.528(3)	C26-C31	1.369(4)	N2-H2A	0.87(3)
C12-H12	0.98	H(2A)••••O(2)	1.98(3)	N(2)-H(2A)••••O(2)	2.675(3)

Table 14
Bond angles (°) for compound **3.**

Bond angles (°)					
C6-C1-C2	117.2(3)	C18-C13-C14	117.3(2)	C29-C28-C27	118.5(4)
C6-C1-C7	121.7(4)	C18-C13-C12	123.3(2)	C29-C28-H28	120.8
C2-C1-C7	121.0(4)	C14-C13-C12	119.4(2)	C27-C28-H28	120.8
C3-C2-C1	121.3(3)	C15-C14-C13	121.0(3)	C28-C29-C30	122.8(3)
C3-C2-H2	119.3	C15-C14-H14	119.5	C28-C29-F2	118.2(4)
C1-C2-H2	119.3	C13-C14-H14	119.5	C30-C29-F2	119.0(4)
C4-C3-C2	120.6(3)	C16-C15-C14	122.1(3)	C29-C30-C31	118.9(3)
C4-C3-H3	119.7	C16-C15-H15	119	C29-C30-H30	120.6
C2-C3-H3	119.7	C14-C15-H15	119	C31-C30-H30	120.6
C5-C4-C3	118.4(3)	C17-C16-C15	116.8(3)	C26-C31-C30	120.2(3)
C5-C4-C8	119.2(2)	C17-C16-C19	121.4(3)	C26-C31-H31	119.9
C3-C4-C8	122.3(2)	C15-C16-C19	121.8(3)	C30-C31-H31	119.9
C6-C5-C4	120.6(3)	C16-C17-C18	121.6(3)	O2-C32-O1	121.3(2)
C6-C5-H5	119.7	C16-C17-H17	119.2	O2-C32-C11	125.2(2)
C4-C5-H5	119.7	C18-C17-H17	119.2	O1-C32-C11	113.5(2)

(*continued on next page*)

Table 14 (*continued*)

Bond angles (°)					
C1-C6-C5	121.8(3)	C13-C18-C17	121.2(3)	O1-C33-C34	110.2(3)
C1-C6-H6	119.1	C13-C18-H18	119.4	O1-C33-H33A	109.6
C5-C6-H6	119.1	C17-C18-H18	119.4	C34-C33-H33A	109.6
C1-C7-H7A	109.5	C16-C19-H19A	109.5	O1-C33-H33B	109.6
C1-C7-H7B	109.5	C16-C19-H19B	109.5	C34-C33-H33B	109.6
H7A-C7-H7B	109.5	H19A-C19-H19B	109.5	H33A-C33-H33B	108.1
C1-C7-H7C	109.5	C16-C19-H19C	109.5	C33-C34-C35	114.4(3)
H7A-C7-H7C	109.5	H19A-C19-H19C	109.5	C33-C34-C36	108.1(3)
H7B-C7-H7C	109.5	H19B-C19-H19C	109.5	C35-C34-C36	113.6(3)
N1-C8-C4	114.5(2)	N1-C20-C25	120.6(2)	C33-C34-H34	106.8
N1-C8-C9	109.31(19)	N1-C20-C21	121.6(2)	C35-C34-H34	106.8
C4-C8-C9	110.1(2)	C25-C20-C21	117.8(2)	C36-C34-H34	106.8
N1-C8-H8	107.6	C22-C21-C20	120.5(3)	C34-C35-H35A	109.5
C4-C8-H8	107.6	C22-C21-H21	119.8	C34-C35-H35B	109.5
C9-C8-H8	107.6	C20-C21-H21	119.8	H35A-C35-H35B	109.5
C10-C9-C8	108.2(2)	C23-C22-C21	119.4(3)	C34-C35-H35C	109.5
C10-C9-H9A	110.1	C23-C22-H22	120.3	H35A-C35-H35C	109.5
C8-C9-H9A	110.1	C21-C22-H22	120.3	H35B-C35-H35C	109.5
C10-C9-H9B	110.1	C24-C23-C22	122.0(3)	C34-C36-H36A	109.5
C8-C9-H9B	110.1	C24-C23-F1	118.8(3)	C34-C36-H36B	109.5
H9A-C9-H9B	108.4	C22-C23-F1	119.2(3)	H36A-C36-H36B	109.5
N2-C10-C11	124.8(2)	C23-C24-C25	119.1(3)	C34-C36-H36C	109.5
N2-C10-C9	119.5(2)	C23-C24-H24	120.4	H36A-C36-H36C	109.5
C11-C10-C9	115.6(2)	C25-C24-H24	120.4	H36B-C36-H36C	109.5
C10-C11-C32	120.4(2)	C24-C25-C20	121.2(3)	C20-N1-C8	119.50(19)
C10-C11-C12	118.1(2)	C24-C25-H25	119.4	C20-N1-C12	121.27(19)
C32-C11-C12	121.3(2)	C20-C25-H25	119.4	C8-N1-C12	119.20(18)
N1-C12-C11	110.56(18)	C31-C26-C27	118.8(3)	C10-N2-C26	125.4(2)
N1-C12-C13	113.52(19)	C31-C26-N2	119.9(3)	C10-N2-H2A	113(2)
C11-C12-C13	112.8(2)	C27-C26-N2	121.2(3)	C26-N2-H2A	119(2)
N1-C12-H12	106.5	C26-C27-C28	120.8(3)	C32-O1-C33	117.5(2)
C11-C12-H12	106.5	C26-C27-H27	119.6	N(2)-H(2A)••••O(2)	136(3)
C13-C12-H12	106.5	C28-C27-H27	119.6		

Table 15
Torsional angles [°] for compound **3.**

Torsional angles [°]					
C6-C1-C2-C3	-0.9(5)	C11-C12-C13-C14	-59.5(3)	C27-C26-C31-C30	0.9(5)
C7-C1-C2-C3	179.2(3)	C18-C13-C14-C15	-0.4(4)	N2-C26-C31-C30	-179.6(3)
C1-C2-C3-C4	-1.1(5)	C12-C13-C14-C15	-179.2(3)	C29-C30-C31-C26	-0.6(6)
C2-C3-C4-C5	1.7(4)	C13-C14-C15-C16	0.6(5)	C10-C11-C32-O2	4.9(4)
C2-C3-C4-C8	-175.6(3)	C14-C15-C16-C17	-0.2(5)	C12-C11-C32-O2	179.8(3)
C3-C4-C5-C6	-0.4(4)	C14-C15-C16-C19	178.3(3)	C10-C11-C32-O1	-175.4(2)
C8-C4-C5-C6	177.0(3)	C15-C16-C17-C18	-0.3(5)	C12-C11-C32-O1	-0.6(3)
C2-C1-C6-C5	2.2(5)	C19-C16-C17-C18	-178.8(3)	O1-C33-C34-C35	57.0(4)
C7-C1-C6-C5	-177.9(3)	C14-C13-C18-C17	-0.1(4)	O1-C33-C34-C36	-175.4(3)
C4-C5-C6-C1	-1.6(5)	C12-C13-C18-C17	178.6(2)	C25-C20-N1-C8	13.7(3)
C5-C4-C8-N1	156.7(2)	C16-C17-C18-C13	0.5(5)	C21-C20-N1-C8	-166.0(2)
C3-C4-C8-N1	-26.1(3)	N1-C20-C21-C22	178.8(2)	C25-C20-N1-C12	-168.5(2)
C5-C4-C8-C9	-79.7(3)	C25-C20-C21-C22	-0.9(4)	C21-C20-N1-C12	11.9(3)
C3-C4-C8-C9	97.5(3)	C20-C21-C22-C23	0.5(4)	C4-C8-N1-C20	-77.7(3)
N1-C8-C9-C10	59.7(3)	C21-C22-C23-C24	0.0(5)	C9-C8-N1-C20	158.3(2)
C4-C8-C9-C10	-66.8(2)	C21-C22-C23-F1	-179.7(3)	C4-C8-N1-C12	104.4(2)
C8-C9-C10-N2	126.7(2)	C22-C23-C24-C25	-0.1(5)	C9-C8-N1-C12	-19.6(3)
C8-C9-C10-C11	-49.4(3)	F1-C23-C24-C25	179.6(2)	C11-C12-N1-C20	152.6(2)
N2-C10-C11-C32	-3.0(4)	C23-C24-C25-C20	-0.3(4)	C13-C12-N1-C20	-79.4(3)
C9-C10-C11-C32	172.9(2)	N1-C20-C25-C24	-178.9(2)	C11-C12-N1-C8	-29.5(3)
N2-C10-C11-C12	-178.0(2)	C21-C20-C25-C24	0.8(4)	C13-C12-N1-C8	98.4(2)
C9-C10-C11-C12	-2.1(3)	C31-C26-C27-C28	-0.1(5)	C11-C10-N2-C26	170.9(3)

(*continued on next page*)

Table 15 (*continued*)

Torsional angles [°]					
C10-C11-C12-N1	42.8(3)	N2-C26-C27-C28	-179.6(3)	C9-C10-N2-C26	-4.8(4)
C32-C11-C12-N1	-132.2(2)	C26-C27-C28-C29	-1.1(6)	C31-C26-N2-C10	-103.8(3)
C10-C11-C12-C13	-85.6(3)	C27-C28-C29-C30	1.4(7)	C27-C26-N2-C10	75.7(4)
C32-C11-C12-C13	99.4(3)	C27-C28-C29-F2	-179.9(3)	O2-C32-O1-C33	-1.7(4)
N1-C12-C13-C18	-5.0(3)	C28-C29-C30-C31	-0.6(6)	C11-C32-O1-C33	178.6(2)
C11-C12-C13-C18	121.8(3)	F2-C29-C30-C31	-179.3(3)	C34-C33-O1-C32	160.5(3)
N1-C12-C13-C14	173.7(2)				

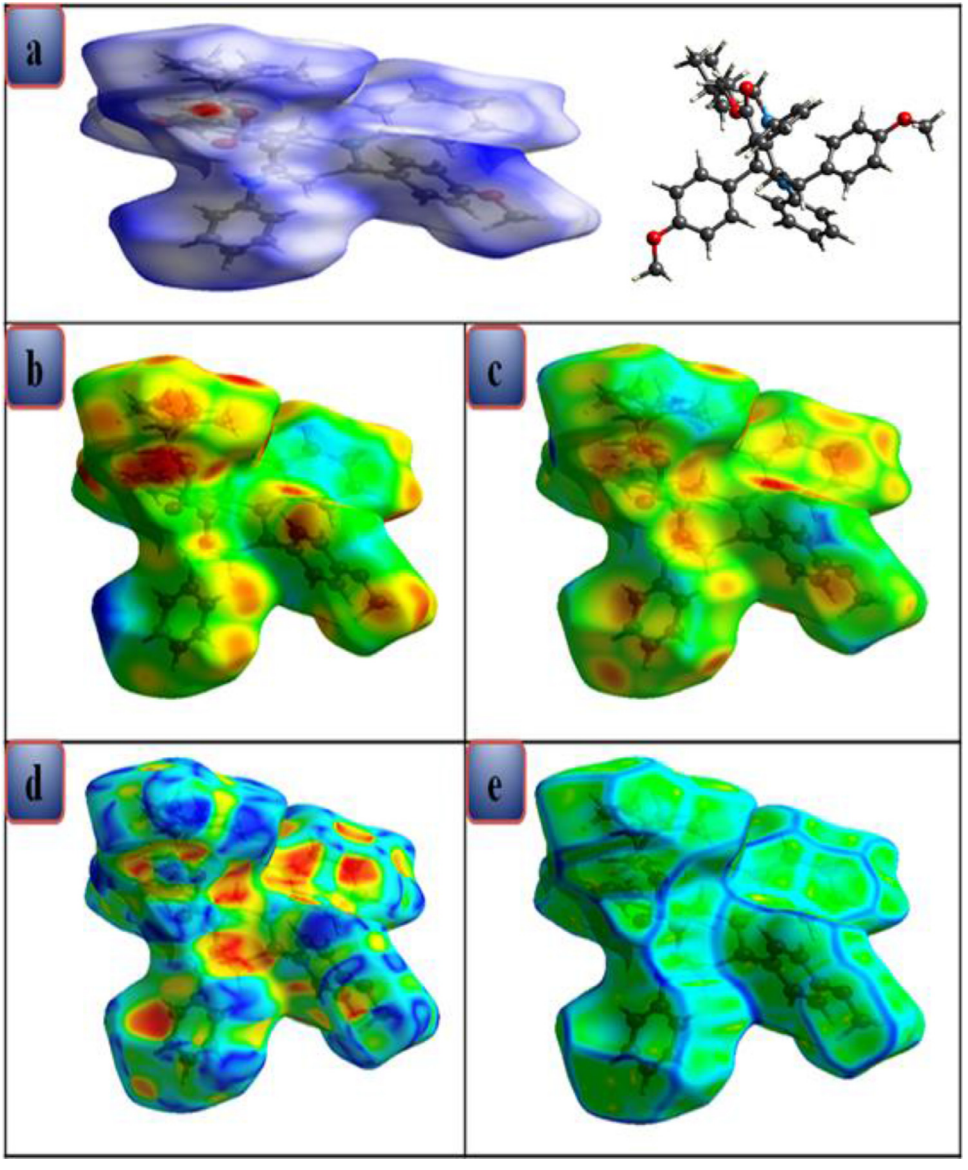

Fig. 3. Hirshfeld surfaces of **1**; (a) d_{norm} (b) d_i (c) d_e (d) Shape index (e) Curvedness.

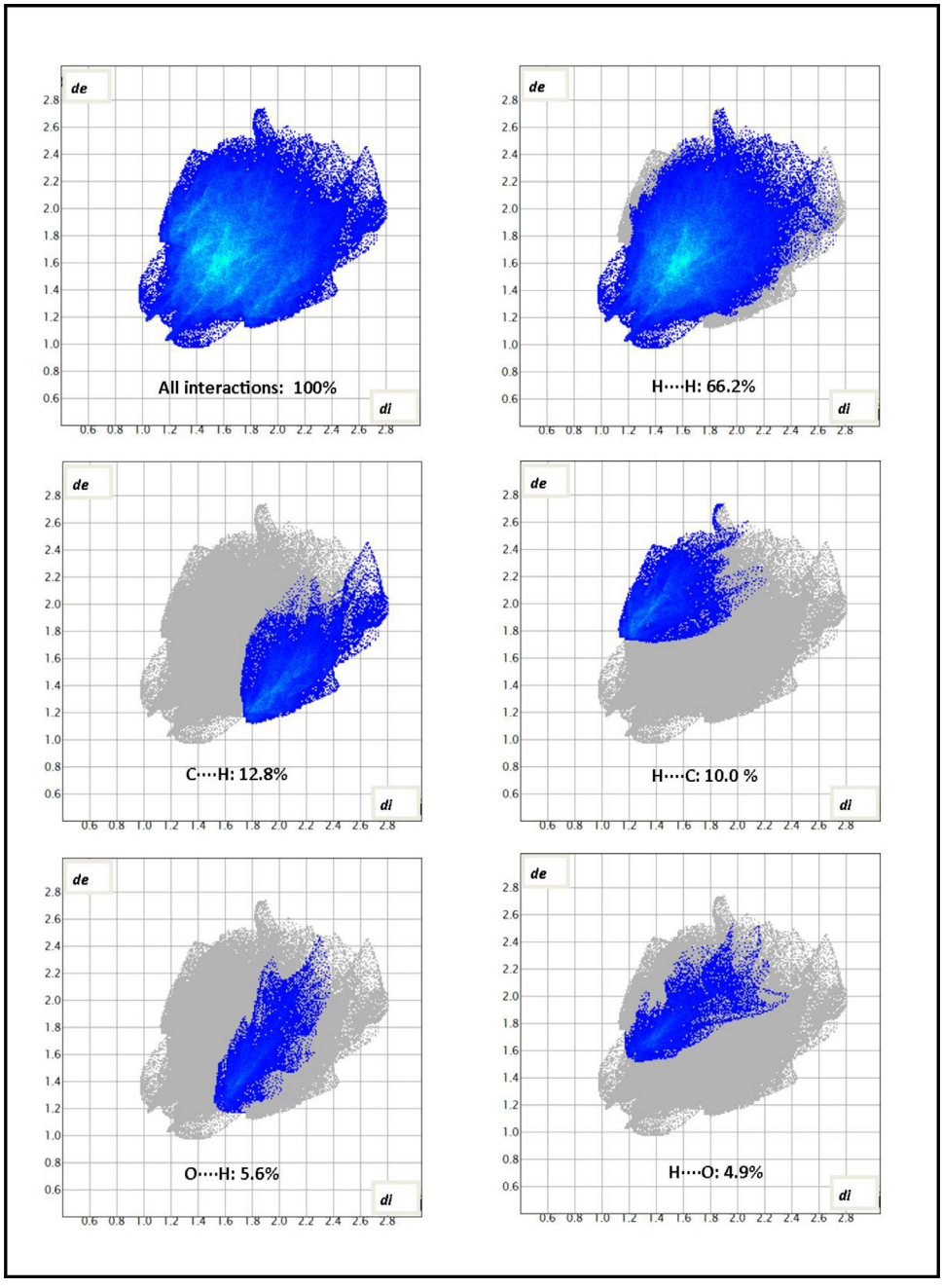

Fig. 4. Finger print plots for **1** (*di* and *de* in Å).

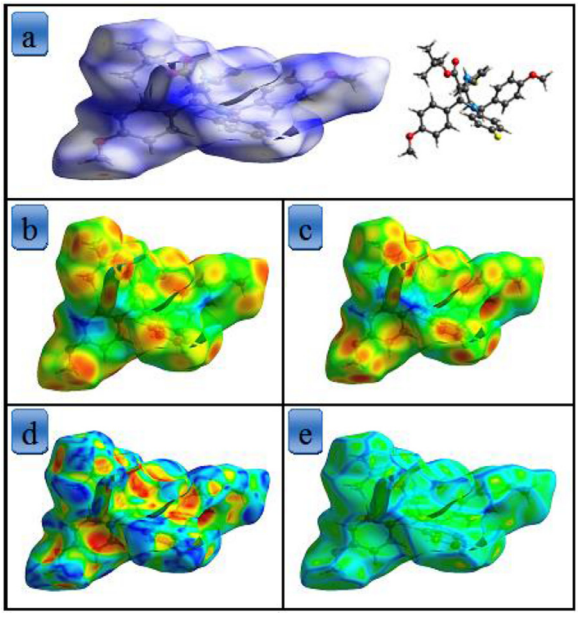

Fig. 5. Hirshfeld surfaces of **2**; (a) d_{norm} (b) d_i (c) d_e (d) Shape index (e) Curvedness.

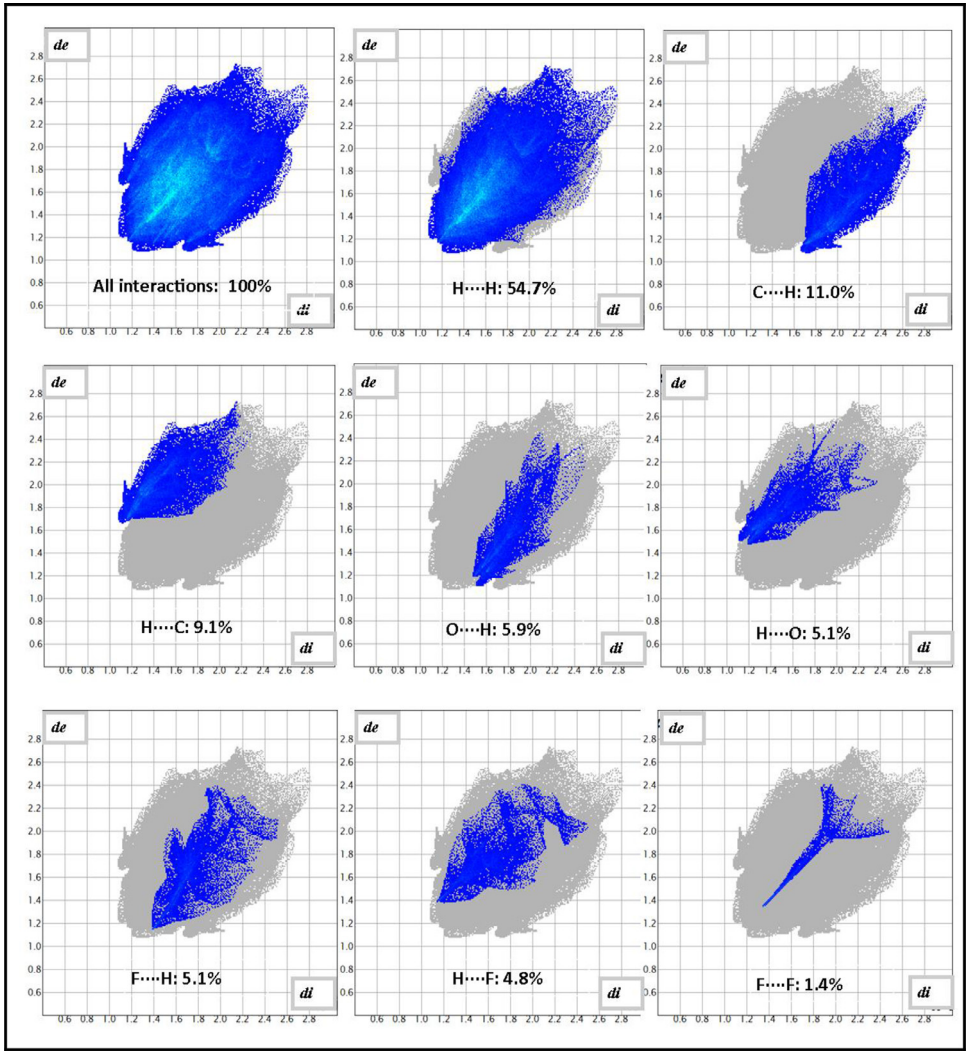

Fig. 6. Finger print plots for **2** (*di* and *de* in Å).

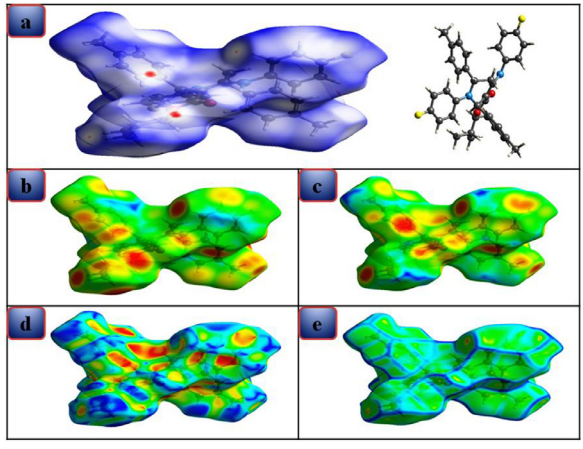

Fig. 7. Hirshfeld surfaces of **3**; (a) d_{norm} (b) d_i (c) d_e (d) Shape index (e) Curvedness.

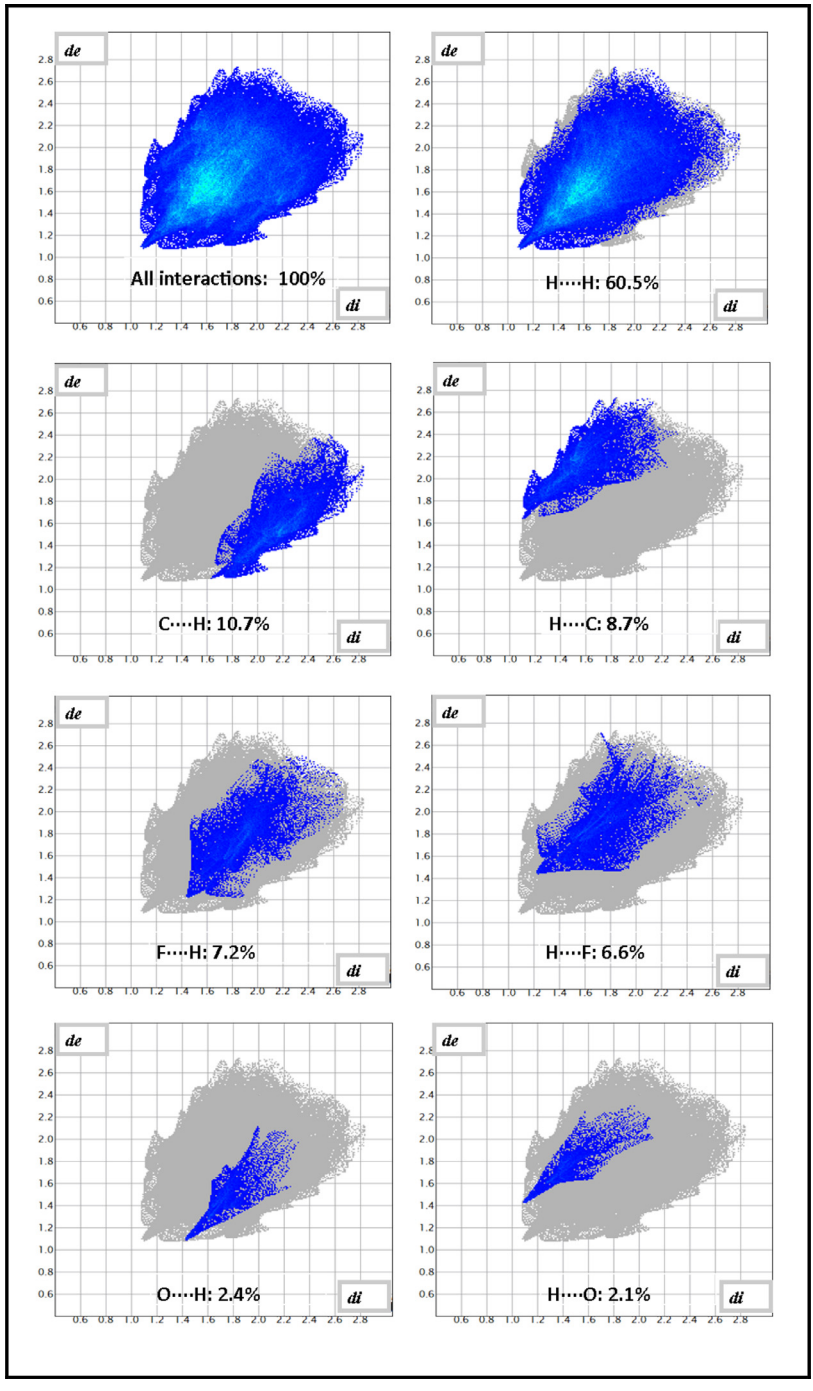

Fig. 8. Finger print plots for **3** (*di* and *de* in Å).

Declaration of Competing Interest

The authors state that they have no known competing financial interests or personal relationships that could have appeared to influence of the work reported in this paper.

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