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X-ray crystal structure analysis of N'-acetyl-N'-phenyl-2-naphthohydrazide

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RESEARCH ARTICLE



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ABSTRACT

N'-Acetyl-*N*'-phenyl-2-naphthohydrazide, a biologically relevant organic molecule, was synthesized following a reported method and characterized based on its single X-ray crystallographic studies. The present manuscript deals with its detailed molecular interactions and X-ray crystal structure. Its space group is *P*-1 with the following unit cell parameters: *a* = 8.9164(7), *b* = 9.7058(9), *c* = 17.7384(12) Å, α = 88.308(7)°, β = 89.744(6)°, γ = 86.744(7)° and *Z* = 2. Crystal structure was solved by direct method and refined by full matrix least squares procedure to a final *R* value of 0.0580 and to a GOOF value of 1.066. The X-ray diffraction analyses showed that the asymmetric unit contains two crystallographically independent molecules. The crystal structure is stabilized by elaborate network of N-H···O and C-H···O hydrogen bonds along with C-H···π and π···π interactions to form supramolecular structures.

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1. Introduction

Hydrazones are important class of biologically potent and pharmaceutically useful organic compounds [1-3]. They find many applications in fluorescent chemosensors [4,5], as auxiliaries in asymmetric synthesis [6], photo switches in photopharmacology [7], and linkers in preparing bifunctional molecules [8-10] and as ligands or directing groups in organic synthesis [11-13].

N,*N*'-Diacylhydrazones are functionalized hydrazone derivatives which are reported to exhibit various biological activities, including antitumor, antidiabetic, anti-inflammation, and anti-infection [14-20]. The title compound, *N*'-acetyl-*N*'-phenyl-2-naphthohydrazide (1) was synthesized following a reported method [21] as shown in Scheme 1, and characterized based on its single X-ray crystallographic studies.

2. Experimental

2.1. General

For crystallization, 50 mg of compound N'-acetyl-N'phenyl-2-naphthohydrazide (**1**) was dissolved in 5 mL DMSO and left for several days at ambient temperature which yielded yellowish block shaped crystals which was suitable for X-ray diffraction analysis, were synthesized following the reported method as described in literature [21].

2.2. Crystal structure determination and refinement

The cell dimensions were determined by least-squares fit of angular settings of 3226 reflections in the θ range 2.27 to 27.97°. The value of $R_{int} = 0.0187$ and $R_{sigma} = 0.0381$ shows satisfactory quality of the data. The molecular structure solution was obtained by direct method procedure as using SHELXT [22]. Six cycles of full-matrix least-squares refinement was carried out and it brought the final *R*-factor to 0.0580 and to GOOF value of 1.066.

All non-hydrogen atoms of the molecule were located in the best *E*-map and refined in anisotropic approximation using SHELXL [22]. The position of all the Hydrogen atoms bonded to carbon atoms were geometrically fixed and allowed to ride on the corresponding non-H atoms (C-H = 0.93-0.96 Å, and U_{iso}(H) = 1.5 U_{eq} of the attached C atoms for methyl groups and 1.2 U_{eq}(C) for other H atoms) except for H12, H35 and H35' atoms attached to nitrogen atoms N12, N35 and N35'. The residual electron density in the final difference Fourier map between -0.27 < $\Delta\rho$ < 0.61. The geometry of the title molecule was calculated using WinGX [23], PARST [24] and PLATON [25] software. Crystallographic data are summarized in Table 1.

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 Table 1. Crystallographic characteristics, details of X-ray data collection, and structure refinement parameters for compound 1.

Empirical formula	C ₁₉ H ₁₆ N ₂ O ₂
Formula weight	304.34
Temperature (K)	150.01(10)
Crystal system	Triclinic
Space group	P-1
a, (Å)	8.9164(7)
b, (Å)	9.7058(9)
c, (Å)	17.7384(12)
α (°)	88.308(7)
β (°)	89.744(6)
γ (°)	86.744(7)
Volume (Å ³)	1531.9(2)
Ζ	4
$\rho_{calc}(g/cm^3)$	1.320
μ (mm ⁻¹)	0.087
F(000)	640.0
Crystal size (mm ³)	$0.3 \times 0.2 \times 0.2$
Radiation	ΜοΚα (λ = 0.71073)
20 range for data collection (°)	4.206 to 51.996
Index ranges	$-10 \le h \le 10, -11 \le k \le 11, -21 \le l \le 12$
Reflections collected	8450
Independent reflections	5935 [R _{int} = 0.0187, R _{sigma} = 0.0381]
Data/restraints/parameters	5935/936/547
Goodness-of-fit on F ²	1.060
Final R indexes $[I \ge 2\sigma(I)]$	$R_1 = 0.0580, wR_2 = 0.1421$
Final R indexes [all data]	$R_1 = 0.0743$, $wR_2 = 0.1579$
Largest diff. peak/hole (e.Å-3)	0.61/-0.27



Scheme 1. Synthesis of N'-acetyl-N'-phenyl-2-naphthohydrazide (1).

3. Results and discussion

The molecular structure containing the atomic labeling of the asymmetric unit of the crystal *N*'-acetyl-*N*'-phenyl-2naphthohydrazide is shown in Figure 2 [26]. The X-ray diffraction analyses showed that the asymmetric unit of compound **1** contains two crystallographically independent molecules *A* and *B*. The molecule consists of a naphthalene ring and a benzene ring connected through a *N*'-acetylformo hydrazide bridge. In molecule *B*, the *N*'-methyl-*N*-phenylaceto hydrazide moiety is disordered over two sites with an occupancy ratio of 0.7531:0.2469.

The geometric parameters, including bond distances and bond angles, show normal geometry [27] and are in close relation to the related structure N-(4-nitrobenzoyl)-N'phenylhydrazine [28]. The length of the N-N single bond between nitrogen atoms is 1.388(2) Å in molecule A and the average value of 1.384 Å in molecule B; this is close to the respective bond length of 1.390(4) Å present in C13H11N3O3. Here, the N-N-C bond angles deviate slightly from the ideal value of 120° by 1.1°, which is due to the presence of substitutions of acetyl groups and carbonyl groups at its ends. In molecule *A*, the acetyl group is *-sc* to the hydrazine moiety as evident from the C11-N12-N13-C14 torsion angle value of -90.0(3)°. The substituent carbonyl groups have an average value of C=O bond length of 1.217 Å, which is very close to its standard value (1.210 Å, [26]). Whereas, the N-N-C bond angle value of 118.7(3)°, the torsion angle value of N2-N1-C7-O7 of -3.3(5)° signifies that carbonyl group is -sp to hydrazine moiety for molecule reported in literature [28]. In both title molecule 1 and the molecule of literature, nearly orthogonal values of torsion angle C-N-N-C signifies tendency of the lone-pair orbitals on nitrogen atoms to reduce the corresponding overlap and resonance integrals [28].

In the naphthalene ring systems, the endocyclic angles at C1, C3, C8 and C8' are narrowed, while those at C2, C6, C26, C27, C29, C32', C31', C29', C26', C26', C27' and C24' are expanded from 120°, respectively. This would appear to be a real effect caused by the fusion of the smaller benzene ring systems by which the strain is taken up by the angular distortion [29]. All the benzene rings are individually planar which is evident from smaller values of torsion angles. In molecule *A*, the benzene ring is twisted with respect to the naphthalene ring at a dihedral angle of $87.01(6)^\circ$. Some of the important bond lengths and bond angles are listed in Table 2. The dihedral angle value of $79.86(0)^\circ$ shows that both the rings of the compound of the literature are also nearly orthogonal to each other [28].

Analysis of the crystal packing showed that there exists a network of N-H···O and C-H···O intermolecular hydrogen bonds. 038 acts as an acceptor atom for two types of hydrogen bonds, by interactions with N12 and C26 through H12 and H26 hydrogen atoms resulting in a relatively stronger C-H…O hydrogen bond. The hydrogen H35 on atom N35 of molecule B forms an intermolecular strong hydrogen bond with the carbonyl atom 015 of molecule A. In addition to this, there exists a wide array of C-H··· π and π ··· π interactions for crystal structure stabilization and to form supramolecular structures. The alkyl-aromatic hydrogen bond connects the parent molecules to their centrosymmetrically related molecules. The 90° angle for stacking rings is observed for 1-1, 1-2, 1-4, 1-5, 2-1, 2-4, 4-1, 4-2, 4-4, 4-5, 5-1, 5-4, and 6-7 molecular pairs. The geometry of these interactions is presented in Tables 3 and 4, respectively. Here Cg/····Cg/ represents the distance between the ring centroids; CgI---P represents the perpendicular distance of the centroid of one ring from the plane of the other; α is the dihedral angle between the planes of rings *I* and *J*; β is the angle between the normal to the centroid of ring *I* and the line joining ring centroids; Δ is the displacement of the centroid of rings *J*

62	1.302(3)		629	630		1.403(0)
C10	1.412(4)		C30	C31		1.352(5)
C11 C2	1.493(3)		C31	C32		1.425(8)
C3	1.431(3)		C32	040		1.412(/)
C9	1.408(3)		C34	040 N2E		1.210(0)
C5	1.400(4)		N32	N36		1.303(0)
C6	1.333(4)		(24)	C25'		1 331(15)
C7	1 341(4)		C24'	(33'		1 446(15)
C8	1.341(4)		C24'	C34'		1.45(3)
C9	1 392(4)		C25'	C26'		1 465(17)
C10	1 370(4)		C26'	C27'		1 374(15)
N12	1 364(3)		C26'	C31'		1 47(3)
017	1 210(3)		C27'	C28'		1.354(15)
C16	1.488(3)		C28'	C29'		1.405(16)
N13	1.356(3)		C29'	C30'		1.346(17)
015	1.223(3)		C30'	C31'		1.42(3)
C19	1.373(3)		C31'	C32'		1.36(3)
C23	1.375(3)		C32'	C33'		1.364(13)
N13	1.434(3)		C34'	040'		1.210(16)
C20	1.385(3)		C34'	N35'		1.367(16)
C21	1.369(4)		N35'	N36		1.36(4)
C22	1.375(4)		C37	C39		1.490(3)
C23	1.380(3)		C37	N36		1.342(3)
N13	1.388(2)		C37	038		1.228(3)
C25	1.415(5)		C41	C42		1.373(3)
C33	1.367(5)		C41	C46		1.376(3)
C34	1.499(8)		C41	N36		1.435(3)
C26	1.356(5)		C42	C43		1.379(3)
C27	1.419(5)		C43	C44		1.374(4)
C28	1.418(6)		C44	C45		1.374(4)
C32	1.401(10)		C45	C46		1.382(3)
Atom	1.363(6)	Angle (°)	Atom	Atom	Atom	Angle (%)
C1	C10	119 0(2)	C20	C21	C22	120 4(5)
C1	C11	117.6(2)	C27	(32	C31	119 2(5)
C1	C11	1734(2)	C27	C32	C33	119.6(6)
C2	C3	123.4(2)	(33	C32	C31	121 2(7)
C3	C2	121.3(2)	C24	C33	C32	120.7(5)
C3	C2	118.4(2)	040	C34	C24	122.4(6)
C3	C4	120 5(2)	040	C34	N25	122 7(7)
		120.5(2)	010	0.5 4	1133	143./[/]
C4	C3	120.3(3)	N35	C34	C24	113.9(6)
C4 C5	C3 C6	120.3(3) 120.0(3)	N35 C34	C34 N35	C24 N36	113.9(6) 118.6(8)
C4 C5 C6	C3 C6 C5	120.3(3) 120.0(3) 121.3(3)	N35 C34 C25'	C34 N35 C24'	C24 N36 C33'	113.9(6) 118.6(8) 121.6(12)
C4 C5 C6 C7	C3 C6 C5 C8	120.3(3) 120.0(3) 121.3(3) 120.5(3)	N35 C34 C25' C25'	C34 N35 C24' C24'	C24 N36 C33' C34'	113.9(6) 118.6(8) 121.6(12) 126.1(14)
C4 C5 C6 C7 C8	C3 C6 C5 C8 C7	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3)	N35 C34 C25' C25' C33'	C34 N35 C24' C24' C24'	N35 C24 N36 C33' C34' C34'	113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13)
C4 C5 C6 C7 C8 C8	C3 C6 C5 C8 C7 C3	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2)	N35 C34 C25' C25' C33' C24'	C34 N35 C24' C24' C24' C25'	C24 N36 C33' C34' C34' C26'	113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12)
C4 C5 C6 C7 C8 C8 C8 C8	C3 C6 C5 C8 C7 C3 C7 C7	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3)	N35 C34 C25' C25' C33' C24' C25'	C34 N35 C24' C24' C24' C24' C25' C25' C26'	C24 N36 C33' C34' C34' C26' C31'	113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13)
C4 C5 C6 C7 C8 C8 C8 C8 C8 C9	C3 C6 C5 C8 C7 C3 C7 C8	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3)	N35 C34 C25' C25' C33' C24' C25' C25' C27'	C34 N35 C24' C24' C24' C25' C25' C26' C26'	C24 N36 C33' C34' C34' C26' C31' C25'	123.7(7) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12)
C4 C5 C6 C7 C8 C8 C8 C8 C9 C10	C3 C6 C5 C8 C7 C3 C7 C8 C1	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2)	C34 C25' C25' C25' C24' C25' C24' C25' C27' C27'	C34 C34 C34 C24' C24' C25' C26' C26' C26'	C24 N36 C33' C34' C34' C26' C31' C25' C31'	113.9(6) 113.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15)
C4 C5 C6 C7 C8 C8 C8 C8 C9 C10 C11	C3 C6 C5 C8 C7 C3 C7 C8 C1 C1	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2)	N35 C34 C25' C25' C33' C24' C25' C27' C27' C27' C28'	C34 C34 N35 C24' C24' C24' C24' C26' C26' C26' C26' C26'	N33 C24 N36 C33' C34' C24' C26' C31' C25' C31' C25' C31'	113.9(6) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12)
C4 C5 C6 C7 C8 C8 C8 C9 C10 C11 C11 C11	C3 C6 C5 C8 C7 C3 C7 C8 C1 C1 C1 C1	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2)	N35 C34 C25' C25' C25' C24' C25' C27' C27' C28' C27' C28' C27'	C34 N35 C24' C24' C24' C24' C26' C26' C26' C26' C26' C26' C26' C27' C28'	C24 N36 C33' C34' C34' C26' C31' C25' C31' C25' C31' C26' C29' C29'	113.9(6) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 102.0(12)
C4 C5 C6 C7 C8 C8 C8 C9 C10 C11 C11 C11 C11	C3 C6 C5 C8 C7 C3 C7 C7 C3 C7 C7 C3 C7 C7 C3 C7 C7 C7 C3 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 123.6(2) 121.5(2)	010 N35 C34 C25' C33' C24' C25' C27' C27' C28' C27' C28' C27' C28' C27' C30'	C34 N35 C24' C24' C24' C25' C26' C26' C26' C26' C26' C27' C28' C29' C29'	C24 N36 C33' C34' C34' C26' C31' C25' C31' C25' C31' C26' C29' C28' C29' C28'	123.7(7) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 101.6(12)
C4 C5 C6 C7 C8 C8 C8 C9 C10 C11 C11 C11 C11 C11 C14	C3 C6 C5 C7 C3 C7 C8 C1 C1 C1 C1 N12 C16	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2)	010 N35 C34 C25' C33' C24' C25' C27' C28' C27' C28' C27' C30' C27' C30' C29'	C34 N35 C24' C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C30'	C24 N36 C33' C34' C34' C26' C31' C25' C31' C25' C31' C26' C29' C28' C28' C31'	123.7(7) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17)
C4 C5 C6 C7 C8 C8 C8 C8 C9 C10 C11 C11 C11 C11 C11 C14 C14	C3 C6 C5 C7 C3 C7 C8 C1 C1 C1 C1 N12 C16 C16 C16	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.5(2) 120.5(2) 120.5(2) 120.5(3) 120.5(3) 120.5(3) 121.5(2) 122.5(2) 120.5(3) 120.5(3) 120.5(3) 121.5(3) 121.5(3) 121.5(3) 121.5(3) 122.5(2) 122.5(2) 120.5(3) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 122.5(2) 123.5(3) 123.5(3) 123.5(3) 123.5(3) 123.5(3) 123.5(3) 124.5(3) 124.5(3) 124.5(3) 125.5(2) 125	010 N35 C34 C25' C33' C24' C25' C27' C30' C29' C30' C29' C30'	C34 N35 C24' C24' C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31'	N36 C24 N36 C33' C34' C34' C26' C31' C26' C27' C31' C26' C29' C28' C31' C26' C31' C26' C29' C28' C31' C26' C29' C28' C31' C26' C31' C26' C30'	123.7(7) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17) 115(2) 120.6(10)
C4 C5 C6 C7 C8 C8 C8 C8 C9 C10 C11 C11 C11 C11 C11 C11 C14 C14 C14 C14	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 C1 N12 C16 C16 N13 C73 C7 C33 C7 C6 C7 C7 C8 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2)	010 N35 C34 C25' C33' C24' C25' C27' C27' C27' C27' C27' C30' C29' C30' C32' C32'	C34 N35 C24' C24' C25' C26' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31'	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C29' C28' C31' C26' C26' C26' C26' C22'	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $125(2)$ $125(2)$
C4 C5 C6 C7 C8 C8 C8 C9 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C18	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 N12 C16 C16 N13 C23 N12	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 124.5(2) 117.3(2) 122.5(2) 122.5(2) 120.2(2) 120.2(2) 120.9(2)	010 N35 C34 C25' C33' C24' C25' C27' C27' C27' C27' C27' C27' C27' C30' C29' C30' C32' C32' C32'	C34 C34 C34 C24' C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31'	133 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31'	123.7(7) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17) 115(2) 120.0(18) 125(2) 122.4(14)
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C11 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2)	N35 C34 C25' C25' C24' C25' C27' C27' C27' C27' C27' C27' C30' C29' C30' C32'	C34 C34 C34 C24' C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C32' C33'	133 C24 N36 C33' C34' C26' C31' C24'	123.7(7) 113.9(6) 118.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17) 115(2) 120.0(18) 125(2) 122.4(14) 119.1(10)
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C18 C18 C18 C19 C19	C3 C6 C5 C8 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2) 119.1(2)	010 N35 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C33' C32' C33' C32' C33' C32' C33' C32' C34'	C34 N35 C24' C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C32' C32' C34' C3	N36 C24 N36 C33' C34' C26' C26' C21' C26' C29' C28' C31' C26' C29' C28' C31' C26' C29' C28' C31' C26' C30' C24' C31' C24' C31' C34' C34' C34' C34' C34' C34' C34' C34	123.7(7) 113.9(6) 113.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17) 115(2) 120.0(18) 125(2) 122.4(14) 119.1(10) 128(2)
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C18 C18 C18 C19 C20	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2)	040 N35 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C32' >	C34 N35 C24' C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C32' C34' C34'	N36 C24 N36 C33' C34' C26' C26' C27' C26' C29' C28' C28' C28' C28' C28' C28' C26' C29' C28' C26' C26' C29' C28' C31' C26' C31' C26' C31' C34' C34' C34' C34' C34' C34' C34' C34	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$
C4 C5 C6 C7 C8 C8 C8 C9 C10 C11 C11 C11 C11 C11 C14 C14 C14 C14 C14	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2)	040 N35 C34 C25' C33' C24' C25' C27' C27' C27' C27' C27' C30' C29' C30' C32' C33' C32' O40' O40' N35'	C34 N35 C24' C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C26' C25' C31' C25' C31' C26' C28' C28' C28' C28' C28' C21' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C25' C31' C26' C26' C31' C25' C31' C26' C26' C31' C25' C31' C26' C28' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C24' C31' C24' C31' C24' C24' C24' C24' C24' C24' C24' C24	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$
C4 C5 C6 C7 C8 C8 C8 C9 C10 C11 C11 C11 C11 C11 C14 C14 C14 C14 C14	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.2(040 N35 C34 C25' C33' C24' C25' C27' C27' C27' C30' C29' C30' C32' C32' C32' O40' N35' N36	C34 N35 C24' C24' C25' C26' C26' C26' C26' C26' C27' C38' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C27' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C30' C31' C24' C24' C34' C24' C34'	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$ $119(3)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.2(2) 119.4(2)	010 N35 C34 C25' C33' C24' C25' C27' C27' C27' C30' C29' C30' C32' C33' C32' C33' C32' O40' N35' N36 N36	C34 N35 C24' C24' C25' C26' C26' C26' C26' C26' C26' C27' C38' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C30' C31' C26' C30' C31' C26' C30' C31' C24' N35' C24' C34' C34' C34'	123.7(7) 113.9(6) 113.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17) 115(2) 120.0(18) 125(2) 122.4(14) 119.1(10) 128(2) 115(2) 117(2) 119(3) 117.6(2)
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.4(2) 120.2(2) 119.4(2) 119.1(19)	N35 N35 C34 C25' C33' C24' C25' C27' C27' C28' C27' C30' C27' C30' C32' C32' C32' C32' C32' O40' N35' N36 N36 O38	C34 N35 C24' C24' C25' C26' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C26' C27' C26' C29' C28' C31' C26' C29' C28' C31' C26' C26' C30' C31' C26' C30' C26' C30' C26' C31' C26' C31' C31' C34' C34' C34' C34' C34' C34' C34' C34	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$ $117(2)$ $117.6(2)$ $122.4(2)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C7 C3 C7 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 119.10(19) 122.75(19)	N35 N35 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C33' C32' C33' C32' C33' C32' C33' C32' O40' N35' N36 N36 O38 O38	C34 N35 C24' C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C32' C33' C34' C34' C34' C34' C34' C37 C37 C37	N36 C34' C34' C34' C26' C31' C25' C31' C26' C31' C24' C34' C34' C34' C34' C34' C34' C39 N36	123.7(7) 113.9(6) 113.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17) 115(2) 122.4(14) 119.1(10) 128(2) 115(2) 117(2) 119(3) 117.6(2) 122.4(2) 122.4(2) 120.6(2) 118.8(12) 122.9(13) 125.9(12)
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C5 C7 C3 C7 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 120.7(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.0(2) 120.2(2) 119.4(2) 122.75(19) 120.6(18)	010 N35 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C33' N36 N36 O38 C42	C34 N35 C24' C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C24' C34' C39 N36 C46	123.7(7) 113.9(6) 113.6(8) 121.6(12) 126.1(14) 112.2(13) 120.5(12) 116.4(13) 122.2(12) 121.4(15) 121.0(12) 118.8(12) 122.9(13) 121.0(17) 115(2) 122.4(14) 119.1(10) 128(2) 115(2) 117(2) 119(3) 117.6(2) 120.8(2) 120.8(2) 118.8(12) 120.8(12)
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C18 C18 C18 C18 C18 C19 C20 C21 C22 C23 N12 N13 N13 N13	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.2(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.2(2) 119.4(2) 119.10(19) 122.75(19) 120.06(18) 116.81(18)	010 N35 C34 C25' C33' C24' C25' C27' C27' C27' C30' C29' C30' C32' C32' C32' C32' C32' O40' N35' N36 O38 O38 C42 C42	C34 N35 C24' C25' C26' C27' C28' C29' C30' C31' C31' C31' C32' C33' C34' C34' C34' C34' C34' C37 C37 C37 C41	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31' C24' C34' C39 C39 C39 C39 C36 C46 N36	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$ $117(2)$ $117.6(2)$ $122.4(2)$ $120.8(2)$ $118.8(2)$
C4 C5 C6 C7 C8 C8 C9 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.2(2) 119.1(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.2(2) 120.2(010 N35 C34 C25' C33' C24' C25' C27' C27' C27' C27' C27' C30' C29' C30' C32' C32' O40' N35' N36 N36 O38 C42 C42 C46	C34 N35 C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C34' C34' C37 C37 C37 C41 C41	N36 C24 N36 C33' C34' C26' C31' C25' C31' C25' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C24' C34' C39 C34' C39 C36 C46 N36	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $117(2)$ $117(2)$ $117(2)$ $119(3)$ $117.6(2)$ $122.4(2)$ $120.8(2)$ $118.8(2)$ $120.3(2)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 120.2(2) 120.9(2) 119.1(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.2(2) 119.1(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 119.1(2) 120.5(19) 120.0(18) 116.81(18) 122.8(4) 119.8(4)	010 N35 C34 C25' C33' C24' C25' C27' C27' C27' C30' C29' C30' C32' C32' C32' O40' 040' N35 N36 O38 O38 C42 C46 C41	C34 N35 C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C31' C32' C33' C34' C34' C34' C34' C34' C34' C34' C34' C37 C37 C37 C41 C41 C41 C42	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C30' C31' C24' C34' C34' C34' C34' C39 C36 N36 C43	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117.6(2)$ $122.4(2)$ $120.0(2)$ $128.8(2)$ $120.8(2)$ $118.8(2)$ $120.3(2)$ $119.5(2)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.0(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.9(2) 118.8(2) 120.2(2) 119.1(2) 120.4(N35 C34 C25' C33' C24' C25' C27' C27' C27' C28' C27' C30' C32' C32' C32' C32' C32' O40' N35' N36 N38 O38 O38 C42 C42 C41 C44	C34 N35 C24' C24' C25' C26' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C30' C31' C26' C30' C31' C24' C34' C39 C39 C39 N36 C43 C42	123.9(6) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $122.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$ $119(3)$ $117.6(2)$ $122.4(2)$ $120.0(2)$ $120.8(2)$ $118.8(2)$ $120.3(2)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C7 C3 C7 C3 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.3(3) 121.3(3) 120.6(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 119.1(2) 120.4(2) 120.4(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(2) 119.1(2) 120.4(040 035 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C33' C33' C32' C33' C33' C34' C44' C45	C34 N35 C24' C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31' C24' C34' C39 N36 C46 N36 C42 C43 C42 C43	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$ $119(3)$ $117.6(2)$ $122.4(2)$ $122.4(2)$ $122.4(2)$ $122.4(2)$ $122.4(2)$ $120.0(2)$ $120.8(2)$ $118.8(2)$ $120.3(2)$ $119.8(2)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C5 C7 C3 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.2(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.2(2) 119.4(2) 120.2(2) 119.4(2) 120.2(2) 119.4(2) 120.2(2) 119.4(2) 122.75(19) 122.75(19) 122.75(19) 122.8(4) 116.81(18) 122.8(4) 119.8(4) 122.8(4) 119.8(4) 120.2(4) 121.2(4)	040 N35 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C33' C34 C45 C44	C34 N35 C24' C25' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C33' C34' N35' C37 C37 C37 C37 C37 C41 C41 C42 C43 C44 C45	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C24' C34' C39 N36 C46 N36 C42 C43 C46	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $125(2)$ $122.4(14)$ $119.1(2)$ $117(2)$ $119(3)$ $117.6(2)$ $122.4(2)$ $120.8(2)$ $118.8(2)$ $120.8(2)$ $118.8(2)$ $120.3(2)$ $119.8(2)$ $120.4(2)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C5 C7 C3 C7 C7 C8 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C23 N13 N13 C23 N13 N13 C23 C23 C22 C23 C22 C23 C22 C23 C22 C23 C22 C34 C1 C1 C27 C22 C25 C24 C27 C25 C25 C24 C27 C25 C25 C25 C25 C25 C25 C25 C25 C25 C26 C27 C26 C22 C22 C22 C25 C25 C25 C25 C25 C25 C22 C22	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 120.2(2) 118.8(2) 120.2(2) 119.1(2) 120.4(2) 120.4(2) 120.2(2) 119.4(2) 120.4(2) 120.2(2) 119.4(2) 120.4(2) 120.6(18) 116.81(18) 122.8(4) 119.8(4) 117.3(5) 120.2(4) 122.1(4)	010 N35 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C33' C32' C33' C32' C33' C32' C33' C32'	C34 N35 C24' C24' C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C31' C25' C31' C25' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C31' C24' C39 C39 C39 C39 C39 C36 C46 N36 C43 C42 C43 C44 C45	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $117(2)$ $117(2)$ $117(2)$ $117(2)$ $117.6(2)$ $122.4(2)$ $120.8(2)$ $118.8(2)$ $120.8(2)$ $118.8(2)$ $120.3(2)$ $119.5(2)$ $120.4(2)$ $119.1(2)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.10(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.2(2) 119.1(2) 120.4(2) 120.2(2) 119.1(2) 120.2(2) 119.1(2) 120.2(2) 119.1(2) 120.2(2) 119.1(2) 120.2(2) 119.1(3) 122.2(4) 122.8(4) 119.8(4) 117.3(5) 120.2(4) 122.1(4) 118.8(2)	040 C25' C25' C25' C27' C30' C29' C30' C32' C33' C32' O40' N35' N36 N36 O38 O38 O38 C42 C42 C44 C41 C44 C41 N35	C34 N35 C24' C25' C26' C26' C26' C27' C28' C29' C30' C31' C32' C37' C37 C37 C37 C41 C41 C42 C43	N36 C24 N36 C33' C34' C26' C31' C25' C31' C25' C31' C26' C31' C24' C39 C39 C36 N36 C43 C43 C44 C45 C41	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $117.6(2)$ $122.4(2)$ $118.8(2)$ $120.8(2)$ $118.8(2)$ $120.8(2)$ $118.8(2)$ $120.8(2)$ $118.8(2)$ $120.8(2)$ $118.8(2)$ $120.8(2)$ $119.5(2)$ $120.8(2)$ $119.5(2)$ $120.8(2)$ $119.8(2)$ $120.4(2)$ $119.1(2)$ $113.6(4)$
C4 C5 C6 C7 C8 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.5(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 120.2(2) 120.9(2) 119.1(2) 120.4(2) 120.0(2) 119.1(2) 120.2(2) 119.10(19) 122.75(19) 120.06(18) 116.81(18) 122.8(4) 119.8(4) 117.3(5) 120.2(4) 121.2(4) 122.1(4)	N35 N35 C24 C25' C33' C24' C25' C27' C27' C28' C27' C30' C29' C30' C32' C32' C32' C32' C32' C32' C32' C32' C32' O40' N35' N36 O38 O38 O38 O38 O38 C42 C42 C42 C44 C41 N35' N35' N35'	C34 N35 C24' C24' C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C24 N36 C33' C34' C26' C31' C25' C31' C26' C31' C26' C31' C26' C31' C26' C31' C26' C30' C31' C26' C30' C31' C26' C30' C31' C26' C30' C31' C24' C39 C39 N36 C43 C42 C43 C42 C43 C42 C43 C44 C45 C41 C41 C41	123.9(6) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$ $117(2)$ $119(3)$ $117.6(2)$ $122.4(2)$ $120.0(2)$ $120.8(2)$ $118.8(2)$ $120.0(2)$ $120.8(2)$ $118.8(2)$ $120.0(2)$ $120.8(2)$ $119.5(2)$ $120.3(2)$ $119.5(2)$ $120.4(2)$ $120.4(2)$ $113.6(4)$ $123.8(14)$
C4 C5 C6 C7 C8 C8 C9 C10 C11 C11 C11 C11 C14 C14 C14 C14 C14 C14	C3 C6 C5 C8 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C7 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	120.3(3) 120.3(3) 120.5(3) 121.3(3) 120.5(3) 117.4(3) 119.6(2) 123.0(3) 120.7(3) 121.0(2) 114.9(2) 123.6(2) 121.5(2) 117.3(2) 122.5(2) 120.9(2) 118.8(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 120.4(2) 122.5(19) 120.6(18) 116.81(18) 122.8(4) 119.8(4) 117.3(5) 120.2(4) 122.1(4) 118.5(4) 119.4(4) 119.4(4)	040 N35 C34 C25' C33' C24' C25' C27' C28' C27' C30' C29' C30' C32' C33' C32' C32' C32' C32' C33' C32 C33' C32 C33' C34 C42 C44 C45 C44 C45 C37 C37	C34 N35 C24' C24' C24' C25' C26' C26' C26' C26' C27' C28' C29' C30' C31' C31' C31' C31' C31' C31' C31' C31	N36 C34 N36 C33' C34' C26' C31' C25' C31' C26' C30' C31' C24' C34' C34' C34' C34' C34' C39 N36 C46 N36 C42 C43 C42 C43 C41 N35	123.7(7) $113.9(6)$ $113.6(8)$ $121.6(12)$ $126.1(14)$ $112.2(13)$ $120.5(12)$ $116.4(13)$ $122.2(12)$ $121.4(15)$ $121.0(12)$ $118.8(12)$ $122.9(13)$ $121.0(17)$ $115(2)$ $120.0(18)$ $125(2)$ $122.4(14)$ $119.1(10)$ $128(2)$ $115(2)$ $117(2)$ $119(3)$ $117.6(2)$ $122.4(2)$ $120.0(2)$ $120.8(2)$ $118.8(2)$ $120.0(2)$ $120.8(2)$ $118.8(2)$ $120.0(2)$ $120.8(2)$ $118.8(2)$ $120.3(2)$ $119.8(2)$ $120.3(2)$ $119.8(2)$ $120.4(2)$ $113.6(4)$ $123.8(14)$ $123.3(4)$
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C11 C11 C14 C14 C14 C18 C18 C18

C19 C20 C21 C22 N12

C24 C24 C24 C25 C26 C27 C27 C28 Atom C2 C2 C10

C1 C4 C8 C8 C5 C4 C7 C6 C3

С9 C9 C10 С9 N12 017

C19 C19 C23 C18 C21 C20 C21 C18 C11 C14 C14 N12 C25 C33 C33 C26 C25 C28 C32 C32 C29 C28

C31

Length (Å)

Table 3. Geometry of inter- and intra-molecular interactions for compound 1 *.

D-H···A	D–H, Å	H···A, Å	D…A, Å	θ(D-H…A), deg	
N12-H12-038 i	0.90(2)	1.92(2)	2.781(2)	159(2)	
N35-H35-015 ⁱⁱ	0.90(2)	1.88(3)	2.747(11)	161(3)	
C26-H26…O38 i	0.93	2.59	3.490(4)	162	
C6-H6…Cg8 ⁱⁱⁱ	0.93	2.83	3.638(3)	146	
C21-H21Cg1 iv	0.93	2.76	3.617(3)	154	
C29-H29Cg3 v	0.93	2.75	3.528(5)	142	
С39-Н39АСд7 и	0.93	2.84	3.531(3)	130	

* Symmetry codes: (i) x, 1+y, z, (ii) x, y, z, (iii) -x, 2-y, 1-z, (iv) -1+x, y, z, (v) 1-x, 1-y, -z, (vi) 1-x, 1-y, 1-z. Cg1, Cg3, Cg7, and Cg8, and represents the center of gravity of the rings (C24A/C25A/C26A/C27A/C32A/C33A), (C41/C42/C43/C44/C45/C46), (C3/C4/C5/C6/C7/C8) and (C18/C19/C20/C21/C22/C23), respectively.

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CgI	CgJ	CgI····CgJ, Å	Cg <i>I…P</i> , Å	α, deg	β, deg	Δ, Å
1	1 ⁱ	3.663	3.490	0.0	17.6	1.11
1	2^i	3.692	3.490	2.3	19.0	1.20
1	4 ^{<i>i</i>}	3.674	3.452	1.1	20.1	1.25
1	5 ^{<i>i</i>}	3.636	3.457	1.1	20.1	1.13
2	1^i	3.692	3.490	2.3	19.0	1.20
2	4^i	3.794	3.428	1.9	24.4	1.64
4	1^i	3.674	3.449	1.1	20.0	1.26
4	2^i	3.794	3.455	1.9	25.4	1.56
4	4 ^{<i>i</i>}	3.939	3.427	0.0	29.5	1.94
4	5 ^{<i>i</i>}	3.507	3.426	1.4	13.6	0.74
5	1^i	3.635	3.440	1.9	18.8	1.26
5	4 ^{<i>i</i>}	3.507	3.409	1.4	12.3	0.81
6	711	3.7686	3.4249	1.70	26.1	1.55

* Symmetric codes: (i) 1-x, 1-y, -z, (i) -x, 2-y, 1-z. Cg1, Cg2, Cg4, Cg5, Cg6 and Cg7 represent the center of gravity of the rings (C24A/C25A/C26A/C32A/C33A), (C27A/C28A/C29A/C30A/C31A/C32A), (C24'/C25'/C26'/C31'/C32'/C33'), (C26'/C27'/C28'/C29'/C30'/C31'), (C1/C2/C3/C8/C9/C10) and (C3/C4/C5/C6/C7/C8), respectively.



Figure 2. The molecular structure of the compound 1.



Figure 3. Packing view of molecules down to *a* and *b*-axis.

relative to the intersection point of the normal to the centroid of ring *I* and the least-squares plane of ring *J*. These π ··· π contacts describe the interactions present between the naphthalene ring and the benzene ring of compound **1**. The packing of the molecule within the unit cell viewed down the *a* and *b*-axis is shown in Figure 3. Molecules are packed together to form infinite layers along the (001) plane. Whereas the crystal packing arrangement for the related compound of the literature is linked to a complex three-dimensional framework structure by a combination of N-H···O, N-H···N, and C-H···O types of intermolecular H-bonds, resulting in sheet-like structure in dearth of other C-H··· π and π ··· π contacts [28].

4. Conclusions

Single crystal X-ray diffraction studies led to unambiguous crystal structure determination of the compound which crystallizes into triclinic crystal system with space group *P*-1. Direct methods were used to solve the crystal structure and refined by full matrix least squares procedure to final *R* value of 0.0580. In molecule *B*, the moiety is disordered over two sites with an occupancy ratio of 0.7521:0.2469. A complete set of intermolecular hydrogen bonds; C-H···π and π ···π interactions was observed and quantified for crystal packing analysis.

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Supporting information S

CCDC-2110780 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via https://www.ccdc.cam.ac.uk/structures/, or by e-mailing data request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033.

Disclosure statement DS

Conflict of interest: The authors declare that they have no conflict of interest. Ethical approval: All ethical guidelines have been adhered. Sample availability: Samples of the compound are available from the author.

CRediT authorship contribution statement CR

Conceptualization: Vivek Kumar Gupta, Goutam Brahmachari; Methodology: Varun Sharma, Indrajit Karmakar; Software: Varun Sharma, Indrajit Karmakar; Validation: Vivek Kumar Gupta, Goutam Brahmachari; Formal Analysis: Vivek Kumar Gupta, Goutam Brahmachari; Investigation: Indrajit Karmakar, Varun Sharma; Resources Vivek Kumar Gupta, Goutam Brahmachari; Data Curation: Varun Sharma, Indrajit Karmakar; Writing -Original Draft: Varun Sharma, Indrajit Karmakar; Writing - Review and Editing: Vivek Kumar Gupta, Goutam Brahmachari; Varun Sharma, Indrajit Karmakar; Visualization: Goutam Brahmachari, Vivek Kumar Gupta; Funding acquisition: none; Supervision: Vivek Kumar Gupta, Goutam Brahmachari.

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