Acta Cryst C STRUCTURAL CHEMISTRY

ISSN 2053-2296

The design of novel metronidazole benzoate structures: exploring stoichiometric diversity

Yara Santiago de Oliveira,[a] Wendell Saraiva Costa,[a] Poliana Ferreira Borges,[b] Maria Silmara Alves de Santana[c] and Alejandro Pedro Ayala[c]*

[a]Department of Pharmacy, Federal University of Ceará, Fortaleza, Ceará, Brazil, [b]Department of Chemical Engineering, Federal University of Ceará, Fortaleza, Ceará, Brazil, and [c]Department of Physics, Federal University of Ceará, Fortaleza, Ceará, Brazil. *Correspondence e-mail: ayala@fisica.ufc.br

Received 12 January 2019
Accepted 20 March 2019

Edited by D. R. Turner, University of Monash, Australia

Keywords: metronidazole benzoate; crystal engineering; cocrystal; salt; physicochemical; crystal structure; pharmaceutical; API; cocrystal.

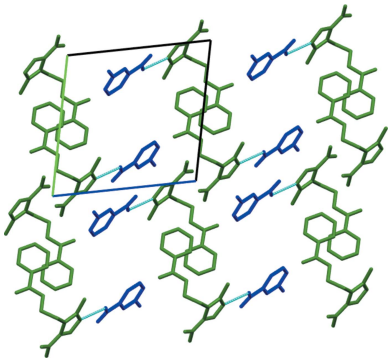
CCDC references: 1890422; 1890421; 1890430; 1890426; 1890432; 1890427; 1890429; 1890433; 1890424; 1890423; 1890428; 1890431; 1890425

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

The use of supramolecular synthons as a strategy to control crystalline structure is a crucial factor in developing new solid forms with physicochemical properties optimized by design. However, to achieve this objective, it is necessary to understand the intermolecular interactions in the context of crystal packing. The feasibility of a given synthon depends on its flexibility to combine the drug with a variety of coformers. In the present work, the imidazole–hydroxy synthon is investigated using as the target molecule benzoylmetronidazole [BZMD; systematic name 2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate], whose imidazole group seems to be a suitable acceptor for hydrogen bonds. Thus, coformers with carboxylic acid and phenol groups were chosen. According to the availability of binding sites presented in the coformer, and considering the proposed synthon and hydrogen-bond complementarity as major factors, different drug–coformer stoichiometric ratios were explored (1:1, 2:1 and 3:1). Thirteen new solid forms (two salts and eleven cocrystals) were produced, namely BZMD–benzoic acid (1/1), $C_{13}H_{13}N_3O_4{\cdot}C_7H_6O_2$, BZMD–$\beta$-naphthol (1/1), $C_{13}H_{13}N_3O_4{\cdot}C_{10}H_8O$, BZMD–4-methoxybenzoic acid (1/1), $C_{13}H_{13}N_3O_4{\cdot}C_8H_8O_3$, BZMD–3,5-dinitrobenzoic acid (1/1), $C_{13}H_{13}N_3O_4{\cdot}C_7H_4N_2O_6$, BZMD–3-aminobenzoic acid (1/1), $C_{13}H_{13}N_3O_4{\cdot}C_7H_7NO_2$, BZMD–salicylic acid (1/1), $C_{13}H_{13}N_3O_4{\cdot}C_7H_6O_3$, BZMD–maleic acid (1/1) {as the salt 1-[2-(benzoyloxy)-ethyl]-2-methyl-5-nitro-1*H*-imidazol-3-ium 3-carboxyprop-2-enoate}, $C_{13}H_{14}N_3O_4^+{\cdot}C_4H_3O_4^-$, BZMD–isophthalic acid (1/1), $C_{13}H_{13}N_3O_4{\cdot}C_8H_6O4$, BZMD–resorcinol (2/1), $2C_{13}H_{13}N_3O_4{\cdot}C_6H_6O_2$, BZMD–fumaric acid (2/1), $C_{13}H_{13}N_3O_4{\cdot}0.5C_4H_4O_4$, BZMD–malonic acid (2/1), $2C_{13}H_{13}N_3O_4{\cdot}C_3H_2O_4$, BZMD–2,6-dihydroxybenzoic acid (1/1) {as the salt 1-[2-(benzoyloxy)ethyl]-2-methyl-5-nitro-1*H*-imidazol-3-ium 2,6-dihydroxybenzoate}, $C_{13}H_{14}N_3O_4^+{\cdot}C_7H_5O_4^-$, and BZMD–3,5-dihydroxybenzoic acid (3/1), $3C_{13}H_{13}N_3O_4{\cdot}C_7H_6O_4$, and their crystalline structures elucidated, confirming the robustness of the selected synthon.

1. Introduction

The understanding of intermolecular interactions in the context of crystal packing and the ability to predict them using supramolecular synthons as a strategy to control crystal structure are key factors in the generation of new solid forms with a desired set of physicochemical properties (Corpinot & Bučar, 2018; Desiraju, 2010). This research area has developed rapidly due to the possibility of rationally designing structures of pharmaceutical compounds (Babu *et al.*, 2012; Blagden *et al.*, 2007; Bolla & Nangia, 2016), improving their physicochemical properties with tailored pharmacokinetics and mechanical properties, such as solubility, stability, flowability and compressibility (Bolla & Nangia, 2016). Further advances have confirmed that the path for the development of a new form depends on clear steps, which are no longer based only



on serendipity, but on the rational design of solid forms as part of a field known as crystal engineering (Kavanagh *et al.*, 2019).

The adopted strategy combines the ability to rationally design supramolecular structures and the modulation of the undesired physicochemical properties of the drug without any covalent modification in the molecules (Berry & Steed, 2017). According to the availability of binding sites present in the coformer, and considering the proposed synthon and hydrogen-bond complementarity as major factors (Wang *et al.*, 2018), different drug–coformer stoichiometric ratios can be explored. Thus, the first step on the development path is to identify and select potential hydrogen-bonding sites in the active pharmaceutical ingredient (API) and to propose appropriate coformers with complementary groups (synthons) (Aitipamula *et al.*, 2014). The initial prospection is vitally important for discovering supramolecular structures with pharmaceutical relevance (Kavanagh *et al.*, 2019; Saha & Desiraju, 2018).

The possibility of generating different solid forms from the API–coformer combination (Berry & Steed, 2017; Cerreia Vioglio *et al.*, 2017; Healy *et al.*, 2017; Shaikh *et al.*, 2018) has consolidated drug development based on pharmaceutical cocrystals, since there is strong scientific evidence corroborating their potential to provide viable candidates for solid formulations having 'by design' properties. Furthermore, a growing interest of the pharmaceutical industry to use these products has been observed, once they are a reality on the market. Thus, we can mention the cocrystals Suglat (ipragliflozin and L-proline), Steglatro (ertugliflozin and L-pyroglutamic acid) and Entresto (valsartan and sacubitril) as successful examples of commercialization (Kavanagh *et al.*, 2019). The growing interest in using pharmaceutical cocrystals have led to the US Food and Drug Administration (FDA, 2018) and the European Medicines Agency (EMA, 2015) publishing position papers related to them. These documents define a regulatory framework, providing guidance to industry and expanding the records for cocrystals.

The target molecule used in this work to apply crystal-design principles was benzoylmetronidazole (BZMD) (Fig. 1), also known as metronidazole benzoate. This drug is indicated for the treatment of infections caused by a wide range of anaerobic, protozoan and bacteroid bacteria, including trichomoniasis, amebiasis, vaginosis and gingivitis (Bempong *et al.*, 2005; Caira *et al.*, 1993). Hoelgaard & Møller (1983) reported two anhydrous (anhydrates I and II) and one monohydrate (BZMDH) form of BZMD, but just the monohydrate and the commercial anhydrous forms have had their crystallographic structures elucidated (Caira *et al.*, 1993). However, none of these structures is reported in the Cambridge Structural Database (CSD; Groom *et al.*, 2016). BZMD anhydrate I crystallizes as blocks or elongated prisms, while the monohydrate form has hexagonally shaped prisms. Both anhydrous forms of BZMD crystallize in triclinic systems, belonging to the $P\overline{1}$ space group but differing in the

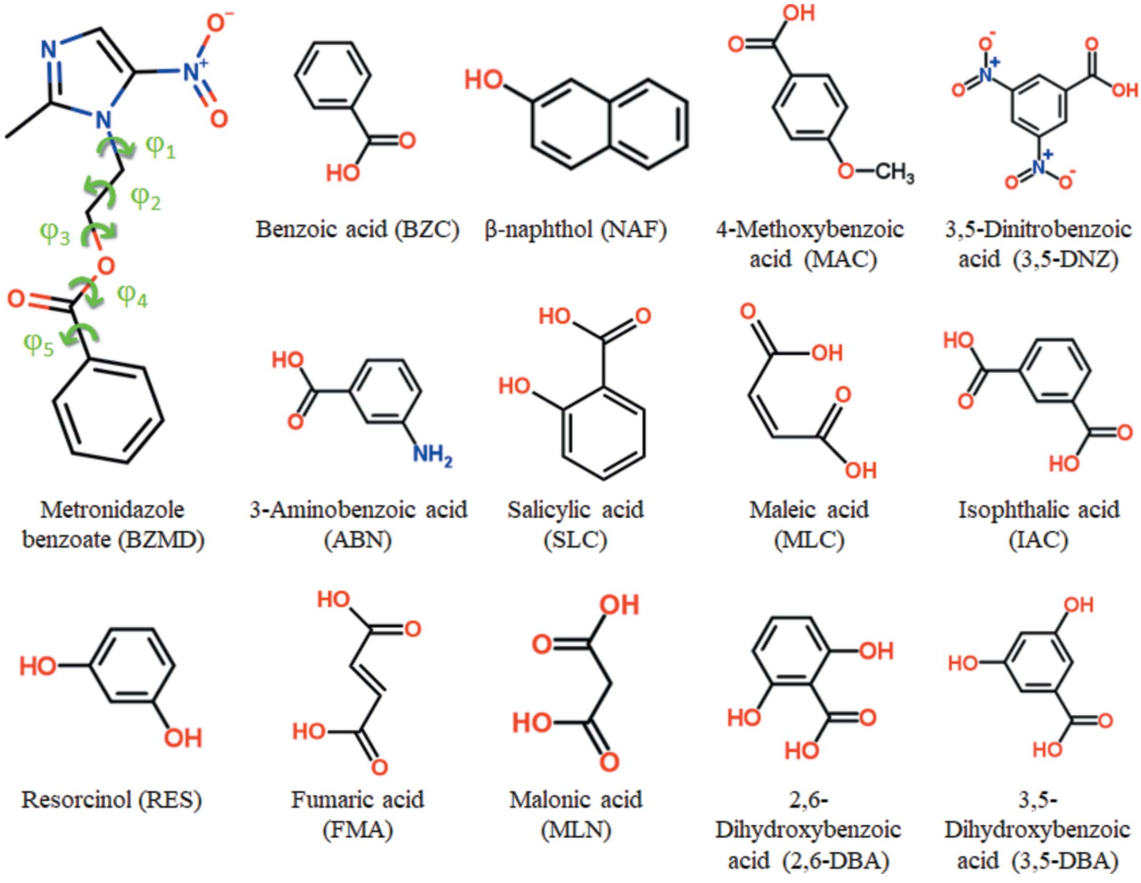


Figure 1
Metronidazole benzoate, cocrystal and salt formers with their corresponding abbreviations. φ_i symbolizes the backbone dihedral angles.

Table 1
Experimental details.

For all determinations, a multi-scan absorption correction (*SADABS*; Bruker, 2016) was used.

	BZMDBZC	BZMDNAF	BZMDMAC	BZMD3,5DNZ	BZMDABN
Crystal data					
Chemical formula	$C_{13}H_{13}N_3O_4{\cdot}C_7H_6O_2$	$C_{13}H_{13}N_3O_4{\cdot}C_{10}H_8O$	$C_{13}H_{13}N_3O_4{\cdot}C_8H_8O_3$	$C_{13}H_{13}N_3O_4{\cdot}C_7H_4N_2O_6$	$C_{13}H_{13}N_3O_4{\cdot}C_7H_7NO_2$
M_r	397.38	419.43	427.41	487.39	412.40
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$
Temperature (K)	300	300	300	300	300
a, b, c (Å)	13.5997 (6), 9.0354 (4), 16.5974 (8)	8.5105 (8), 22.387 (2), 11.7752 (11)	9.1309 (4), 11.1274 (4), 11.8538 (5)	21.0988 (13), 8.4322 (5), 12.0341 (8)	7.9316 (7), 11.9585 (12), 12.1978 (12)
α, β, γ (°)	90, 108.646 (2), 90	90, 108.664 (4), 90	107.365 (1), 103.270 (1), 110.091 (1)	90, 99.505 (2), 90	76.362 (3), 78.927 (3), 79.583 (3)
V (Å^3)	1932.42 (15)	2125.4 (3)	1002.73 (7)	2111.6 (2)	1092.21 (18)
Z	4	4	2	4	2
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.86	0.78	0.11	0.13	0.09
Crystal size (mm)	0.8 × 0.2 × 0.2	0.42 × 0.09 × 0.07	0.73 × 0.49 × 0.21	0.46 × 0.40 × 0.06	0.91 × 0.09 × 0.05
Data collection					
Diffractometer	Bruker APEXII CCD	Bruker D8 VENTURE Kappa Duo PHOTON II CPAD	Bruker APEX3 micro-source	Bruker APEXII CCD	Bruker APEXII CCD
T_{min}, T_{max}	0.675, 0.753	0.678, 1.000	0.587, 0.746	0.587, 0.746	0.587, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	60527, 3542, 2669	39131, 3884, 2810	32021, 4583, 3795	71598, 4820, 3321	38219, 5008, 2711
R_{int}	0.053	0.084	0.063	0.108	0.090
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.603	0.603	0.650	0.650	0.649
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.130, 1.07	0.058, 0.193, 1.06	0.059, 0.165, 1.05	0.065, 0.213, 1.14	0.054, 0.168, 1.01
No. of reflections	3542	3884	4583	4820	5008
No. of parameters	339	365	364	385	340
No. of restraints	0	0	0	0	0
H-atom treatment	All H-atom parameters refined	All H-atom parameters refined	All H-atom parameters refined	All H-atom parameters refined	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.14	0.30, −0.23	0.76, −0.24	0.40, −0.35	0.25, −0.19

	BZMDSLC	BZMDMLC	BZMDIAC	BZMDFMA	BZMD2,6DBA
Crystal data					
Chemical formula	$C_{13}H_{13}N_3O_4{\cdot}C_7H_6O_3$	$C_{13}H_{14}N_3O_4^+{\cdot}C_4H_3O_4^-$	$C_{13}H_{13}N_3O_4{\cdot}C_8H_6O_4$	$C_{13}H_{13}N_3O_4{\cdot}0.5C_4H_4O_4$	$C_{13}H_{14}N_3O_4^+{\cdot}C_7H_5O_4^-$
M_r	413.38	391.33	441.39	333.30	429.38
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Temperature (K)	301	302	304	300	301
a, b, c (Å)	9.5055 (6), 31.2239 (19), 6.8578 (4)	43.130 (3), 5.7944 (4), 15.2645 (11)	8.8300 (3), 33.7182 (10), 7.3199 (2)	9.0358 (5), 26.6419 (14), 6.8796 (3)	8.2443 (4), 15.9009 (7), 15.4526 (8)
α, β, γ (°)	90, 102.628 (2), 90	90, 109.600 (3), 90	90, 107.878 (1), 90	90, 102.419 (2), 90	90, 102.454 (2), 90
V (Å^3)	1986.2 (2)	3593.7 (5)	2074.13 (11)	1617.38 (14)	1978.04 (17)
Z	4	8	4	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.11	0.12	0.11	0.11	0.11
Crystal size (mm)	0.68 × 0.24 × 0.16	0.57 × 0.23 × 0.05	0.95 × 0.3 × 0.11	0.63 × 0.17 × 0.17	0.83 × 0.67 × 0.27
Data collection					
Diffractometer	Bruker D8 VENTURE Kappa Duo PHOTON II CPAD	Bruker D8 VENTURE Kappa Duo PHOTON II CPAD	Bruker D8 VENTURE Kappa Duo PHOTON II CPAD	Bruker APEXII CCD	Bruker D8 VENTURE Kappa Duo PHOTON II CPAD
T_{min}, T_{max}	0.706, 0.746	0.261, 0.746	0.649, 0.746	0.620, 0.746	0.490, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	69959, 4553, 3883	20803, 4130, 2159	38842, 6344, 4809	46849, 3705, 2625	27674, 4348, 3408

Table 1 (continued)

	BZMDSLC	BZMDMLC	BZMDIAC	BZMDFMA	BZMD2,6DBA
R_{int}	0.035	0.089	0.037	0.066	0.076
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.650	0.715	0.650	0.651
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.115, 1.06	0.056, 0.147, 1.02	0.050, 0.145, 1.04	0.051, 0.151, 1.05	0.069, 0.185, 1.10
No. of reflections	4553	4130	6344	3705	4348
No. of parameters	347	322	365	267	356
No. of restraints	100	0	0	0	0
H-atom treatment	All H-atom parameters refined	All H-atom parameters refined	All H-atom parameters refined	H atoms treated by a mixture of independent and constrained refinement	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.20	0.18, −0.22	0.20, −0.21	0.39, −0.33	0.37, −0.27

	BZMD3,5DBA	BZMDRES	BZMDMLN
Crystal data			
Chemical formula	$3C_{13}H_{13}N_3O_4{\cdot}C_7H_6O_4$	$2C_{13}H_{13}N_3O_4{\cdot}C_6H_6O_2$	$2C_{13}H_{13}N_3O_4{\cdot}C_3H_2O_4$
M_r	979.91	660.63	652.57
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, *Pbca*	Orthorhombic, *Pbcn*
Temperature (K)	300	300	300
a, b, c (Å)	7.1481 (2), 36.7892 (8), 18.0584 (4)	26.3241 (4), 7.1612 (1), 33.8433 (5)	26.1542 (4), 7.2708 (1), 16.6719 (3)
α, β, γ (°)	90, 100.451 (1), 90	90, 90, 90	90, 90, 90
V (Å^3)	4670.1 (2)	6379.87 (16)	3170.36 (9)
Z	4	8	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.91	0.88	0.92
Crystal size (mm)	0.28 × 0.14 × 0.06	0.25 × 0.12 × 0.11	0.46 × 0.29 × 0.13
Data collection			
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD	Bruker APEXII CCD
T_{min}, T_{max}	0.835, 0.986	0.623, 0.753	0.736, 0.907
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	56516, 8547, 5499	121051, 5865, 4816	54755, 2893, 2423
R_{int}	0.058	0.066	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.604	0.603	0.602
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.176, 1.01	0.048, 0.147, 1.03	0.078, 0.268, 1.13
No. of reflections	8547	5865	2893
No. of parameters	844	540	244
No. of restraints	1	0	36
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.22	0.30, −0.31	0.33, −0.27

Computer programs: *APEX3* (Bruker, 2012), *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Version 3.10; Macrae *et al.*, 2008) and *VEGA* (Pedretti *et al.*, 2004).

crystal packing and BZMD conformation. The crystalline structure of anhydrate I is mainly determined by C—H···π interactions and weak hydrogen bonds; among them it is relevant to emphasize the role of the N atom of the imidazole group as an acceptor. This fact is evident in the monohydrated form, as the simplest multicomponent BZMD structure, where water molecules act as bridges through O*W*—H···N and O*W*—H···O hydrogen bonds (Caira *et al.*, 1993). Based on these structures, the imidazole group seems to be a suitable acceptor for hydrogen bonds with coformers containing hydroxy groups. Thus, we decided to explore this synthon by choosing coformers with carboxylic acid and phenol groups.

Additional factors, such as solvent, temperature and methodology, also influence the final product (Aitipamula *et al.*, 2014; Sarraguça *et al.*, 2016). Several methods can be used in order to obtain new solid forms (Delori *et al.*, 2012; Do & Friscic, 2017; Douroumis *et al.*, 2017; Hasa & Jones, 2017; James *et al.*, 2012). In this study, the rational design provided by crystal engineering was aligned to the traditional solvent-evaporation methodology (Barikah, 2018), which has been applied successfully with a large number of APIs (Diniz *et al.*, 2018; Sarkar & Rohani, 2015; Shayanfar & Jouyban, 2014; Shayanfar *et al.*, 2014). Following this strategy, thirteen new solid forms (two salts and eleven cocrystals) were obtained successfully employing crystal engineering principles by selecting suitable coformers (Fig. 1).

2. Experimental

2.1. Materials

Metronidazole benzoate was used as received from Brazilian Pharmacopeia (Brazil), whereas the coformers were

purchased from Sigma–Aldrich [2,6-dihydroxybenzoic acid (2,6DBA), 3,5-dihydroxybenzoic acid (3,5DBA), 3,5-dinitrobenzoic acid (3,5DNZ), isophthalic acid (IAC), 4-methoxybenzoic acid (MAC) and resorcinol (RES)], Vetec [benzoic acid (BZC), salicylic acid (SLC), malonic acid (MLN) and 3-aminobenzoic acid (ABN)], Dinâmica [fumaric acid (FMA) and maleic acid (MLC)] and Merck (β-naphthol and NAF). The solvent was purchased from Vetec and used without further purification.

2.2. Solution growth of single crystals

Slow evaporation (Barikah, 2018) was used to grow single crystals, using about 15 mg of metronidazole benzoate, the corresponding amount of the selected coformer and 2 ml of ethanol as solvent. The API–coformer stoichiometric ratio used was based on the number of OH groups present in each coformer. Therefore, the API–coformer ratio for BZC, NAF, MAC, 3,5DNZ and ABN was 1:1, for SLC, MLC, IAC, RES, FMA and MLN was 2:1, and for 2,6DBA and 3,5DBA was 3:1. The vials were left stirring on a hot plate. The solvent was then allowed to evaporate at room temperature. Crystals were harvested after one week.

Seven letter codes were given for the salts and cocrystals obtained, and they are used throughout this article. The first four letters are related to the drug benzoylmetronidazole [BZMD; systematic name 2-(2-methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate] and the last three letters identify the coformer. The title compounds are thus BZMD–benzoic acid (BZMDBZC), BZMD–β-naphthol (BZMDNAF), BZMD–4-methoxybenzoic acid (BZMDMAC), BZMD–3,5-dinitrobenzoic acid (BZMD3,5DNZ), BZMD–3-aminobenzoic acid (BZMDABN), BZMD–salicylic acid (BZMDSLC), BZMD–maleic acid (BZMDMLC), BZMD–isophthalic acid (BZMDIAC), BZMD–resorcinol (BZMDRES), BZMD–fumaric acid (BZMDFMA), BZMD–malonic acid (BZMDMLN), BZMD–2,6-dihydroxybenzoic acid (BZMD2,6DBA) and BZMD–3,5-dihydroxybenzoic acid (BZMD3,5DBA). BZMDBZC, BZMDSLC, BZMDMLC, BZMDIAC, BZMDFMA, BZMDMLN and BZMD3,5DBA crystallized as colourless prisms, whereas BZMDMAC, BZMD3,5DNZ and BZMDABN crystallized as colourless plates. Yellow prism-shaped crystals were obtained for BZMDNAF, BZMDRES and BZMD2,6DBA. Other coformers containing carboxylic acid and phenol functional groups were tested, but only those whose structure was determined are reported in this work. A list of those coformers and the conditions used in the unsuccessful crystallization attempts is given in the supporting information.

2.3. Single-crystal X-ray diffraction

Crystal data, data collection and structure refinement details are summarized in Table 1.

In general, H atoms were located in difference Fourier maps and refined isotropically. In some methyl groups and disordered groups, the corresponding H-atom positions were calculated geometrically and refined using the riding model. For BZMDABN, residual electron densities were observed in solvent-accessible voids associated with disordered solvent molecules and were treated with the *PLATON*/SQUEEZE program (Spek, 2009, 2015).

3. Results

3.1. Structures

The Cambridge Structural Database (CSD, Version 5.40 of 2018; Groom *et al.*, 2016) contains over 900000 entries for small-molecule organic and metal–organic crystal structures. In a general search performed on this database, the synthon Imidazole–HOC produces 1554 hits, whereas Imidazole–carboxylic and Imidazole–phenol were found in 714 and 187 structures, respectively. Thus, the prevalence of synthons relating the imidazole group to carboxylic and phenol moieties are, respectively, 50 and 10%, confirming that they can be used as markers in coformer selection. Based on that, this work follows the pre-established sequence depicted in the *Introduction*, where the first step was the selection of suitable coformers having complementary hydrogen bonds with the API through the proposed imidazole–hydroxy synthon (Im–HO).

3.1.1. Single donor coformers. According to the statistical analysis of the compatible molecular functional groups related to the chosen bonding site of the API, the synthon Im–HO was considered suitable. Thus, in order to verify the previous proposal, coformers with a single hydroxy donor were selected. Multicomponent structures with a 1:1 stoichiometry were produced successfully with BZC, NAF, MAC, 3,5DNZ and ABN. The corresponding crystalline structures are presented in Figs. 2 and 3, which can be classified as cocrystals considering the usual definition for this supramolecular organization (Aitipamula *et al.*, 2014; Dalpiaz *et al.*, 2017). These results demonstrate the practical feasibility of the proposed synthon, but it is also interesting to discuss the main features of the crystal packing of each cocrystal. All the interactions that help to stabilize the novel structures are listed in Table S2 of the supporting information.

It is interesting to consider, firstly, a simple carboxylic acid (BZC) and phenol (NAF), with one hydroxy group each. The crystal packing presented in Fig. 2 shows that the stronger intermolecular interaction in these structures is the imidazole–hydroxy synthon. The shape of the assembled molecules gives us a better understanding of the long-range order (Corpinot & Bučar, 2018). In the case of BZMDBZC (Fig. 2*a*), the Im$\cdots$H—O interaction is the stronger one [1.67 (3) Å], but a weaker interaction involving the BZMD methyl group and the carbonyl group from the carboxylic acid moiety [2.51 (4) Å] defines an $R_2^2(8)$ ring structure (Fig. S2 in the supporting information). BZMD and BZC form intercalated columns around the screw axis laterally linked by the previously described synthon (Fig. 2*a*). The Im$\cdots$H—O contact is also the strongest interaction [1.90 (4) Å], linking BZMD to the NAF coformer. In BZMDNAF (Fig. 2*b*), the planes of the BZMD dimers, defined by a C6—H2*B*$\cdots$O2 homosynthon [2.61 (4) Å], are intercalated with the planes of NAF molecules (Fig. 2*b*).

Cocrystals with a 1:1 stoichiometry were also obtained with the carboxylic acids MAC (Fig. 2*c*) and 3,5DNZ (Fig. 2*d*). In the first, the API and coformer form the same $R_2^2(8)$ synthon observed in BZMDBZC (Fig. S3 in the supporting information), with similar donor–acceptor distances to those in Im···H—O [1.88 (4) Å] and carbonyl–methyl [2.58 (3) Å] interactions. Regarding the crystal packing, BZMD–MAC dimers lie in (120) planes (Fig. 2*c*), which are stacked by π–π interactions between the imidazole and phenyl rings from MAC [3.6911 (13) Å] and BZMD [4.0761 (15) Å]. In BZMD-3,5DNZ, the 3,5DNZ molecule, linked by the target synthon [1.65 (4) Å], is turned 62° from the plane defined by the imidazole group. Furthermore, the API and coformer are also organized in layers (Fig. 2*d*) along the *a* axis, where the 3,5DNZ molecules are flipped consecutively up and down along the *c* axis as a consequence of the glide plane.

Fig. 3 shows the crystalline structure of BZMDABN, which is also defined as a carboxylic acid coformer. Different from the packing observed with other coformers and the same donor moiety, the Im···H—O interaction can be identified [1.72 (4) Å], but the synthon is not observed. This is not the only interesting feature in BZMDABN, since large channels running along the *a* axis are formed. This cavity is surrounded by four molecules (two APIs and two coformers), and a solvent/guest molecule could be present, characterizing an inclusion compound (Peraka *et al.*, 2017). Some residual charges were identified during the structure resolution, which could be associated with nonstoichiometric disordered residual solvent. However, the low concentration of the solvent hindered the determination of a reliable model. The SQUEEZE method (Spek, 2015) implemented in *PLATON* (Spek, 2009) was applied to treat the residual charges, confirming the existence of a solvent-accessible volume of 135 Å^3 and 20 electrons, suggesting the presence of disordered ethanol, as expected considering the crystal-growing method.

3.1.2. Dual donor coformers. The previous results proved the success of the employed strategy based on the Im–HO synthon. Using the same rational design, we proposed to combine the API with coformers containing two binding sites in order to explore the production of solid forms with a 2:1 stoichiometry. In this sense, carboxylic acids and phenols with two hydroxy groups were selected. Figs. 4 and 5 show the crystal packing of the new structures.

Fig. 4 shows the crystal packing of the multicomponent forms obtained using SLC, IAC and MLC. BZMDSLC and BZMDIAC are cocrystals, whereas BZMDMLC is a salt, as

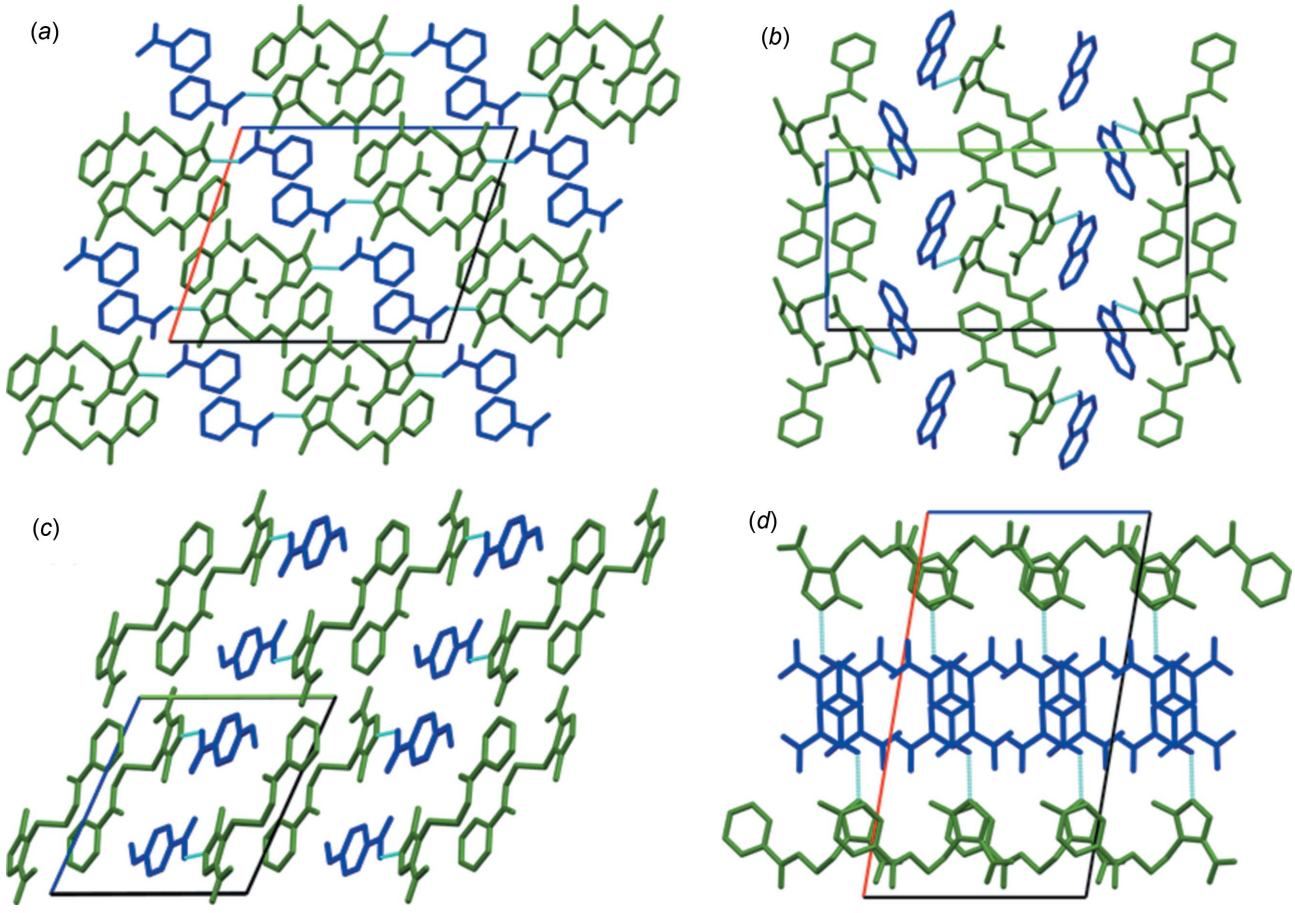


Figure 2
Projection of the crystal packing of (*a*) BZMDBZC (*b* axis), (*b*) BZMDNAF (*a* axis), (*c*) BZMDMAC (*a* axis) and (*d*) BZMD3,5DNZ (*b* axis). H atoms have been omitted for clarity. BZMD is represented in green and coformers in blue. Lattice axes *a*, *b* and *c* are colour-coded red, green and blue, respectively.

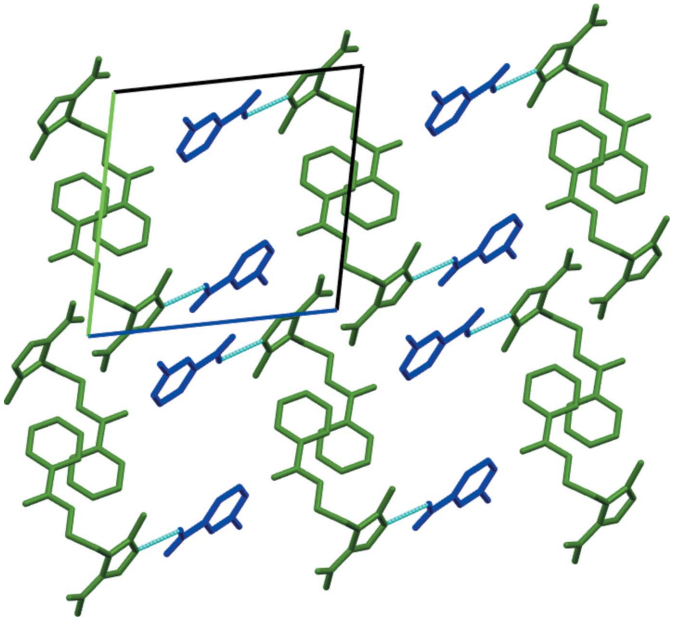


Figure 3
Projection of the crystal packing of BZMDABN (*a* axis), showing the solvent-accessible voids. H atoms have been omitted for clarity. BZMD is represented in green and coformers in blue. Lattice axes *a*, *b* and *c* are colour-coded red, green and blue, respectively.

may be verified in the ellipsoid plot included in the supporting information. Despite the fact that these coformers have two hydroxy groups, they all crystallize with a 1:1 stoichiometry. In order to understand the reasons that lead to the failure of the crystal-design strategy, it is important to discuss in detail the crystal packing of these forms.

The projection of the BZMDSLC structure along the *a* axis shows the API and coformer intercalated columns resembling previously discussed cocrystals (Fig. 4*a*). The carboxy hydroxy group is involved in the Im···H—O interaction [1.76 (2) Å], but the second OH group of SLC does not exhibit the expected supramolecular synthon because it forms an intramolecular hydrogen bond with the carbonyl group. A similar result was obtained for the BZMDMLC salt (Fig. 4*b*). Even considering the charge transfer from one of the carboxylic acid groups of MLC, the same binding site is the stronger intermolecular interaction, forming an $Im^{+}\cdots O$ contact [1.65 (3) Å]. As in BZMDSLC, the second carboxylic acid group, which is still protonated, is linked to the first carbonyl group by an intramolecular interaction thus hindering the formation of the target hydrogen bond. A common factor in SLC and MLC is that both carbonyl groups are close enough to form intramolecular hydrogen bonds, which is more favourable than the Im–HO synthon.

The IAC coformer seems to be a good candidate to avoid the previous problem because the hydroxy groups cannot form an intramolecular contact. However, a 1:1 cocrystal was obtained (Fig. 4*c*), where one of the hydroxy groups forms the Im···H—O interaction [1.79 (3) Å], but the second OH group is involved in a hydrogen bond with another IAC molecule [O—H···O = 1.63 (3) Å]. The strongly linked IAC dimers are bonded to BZMD, forming intercalated antiparallel ribbons and defining the long-range ordering of the BZMDIAC cocrystal. IAC molecules are linked by a carboxylic acid homosynthon forming an $R_2^2(8)$ ring, which is quite prevalent in carboxylic acids. Thus, it is not surprising to observe this kind of synthon in carboxylic acids, but different from the highly probable intramolecular interactions in SLC and MLC, it is not possible to predict them. Thus, from the point of view of crystal design, in order to obtain higher stoichiometric ratios, the main strategy should be to avoid coformers prone to having the selected binding sites involved in intramolecular interactions.

Based on previous results, a phenol (RES) and two carboxylic acids (FMA and MLN) were tested. Fig. 5 shows the crystal packing observed in these new solid forms, which are cocrystals with a 2:1 stoichiometry. The RES coformer fulfills the requirements of our crystal-design strategy, that is, multiple separated hydroxy groups not forming intramolecular hydrogen bonds. Thus, the two donor sites are linked to non-equivalent BZMD molecules by Im···H—O interactions [1.78 (4) and 1.81 (4) Å], giving rise to the

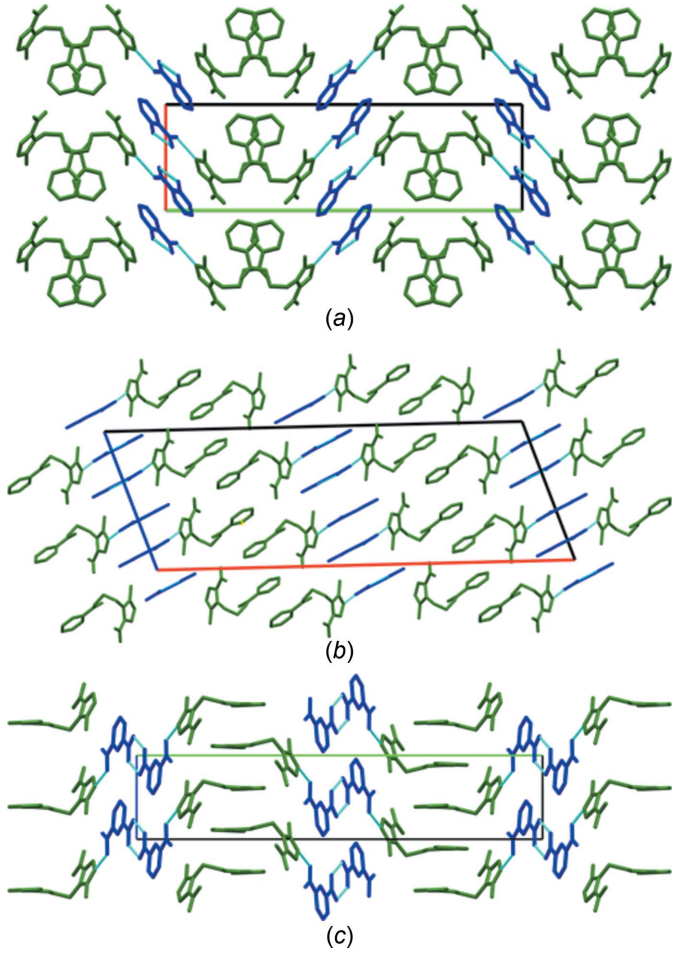


Figure 4
Projection of the crystal packing of (*a*) BZMDSLC (*c* axis), (*b*) BZMDMLC (*b* axis) and (*c*) BZMDIAC (*c* axis). H atoms have been omitted for clarity. BZMD is represented in green and coformers in blue. Lattice axes *a*, *b* and *c* are colour-coded red, green and blue, respectively.

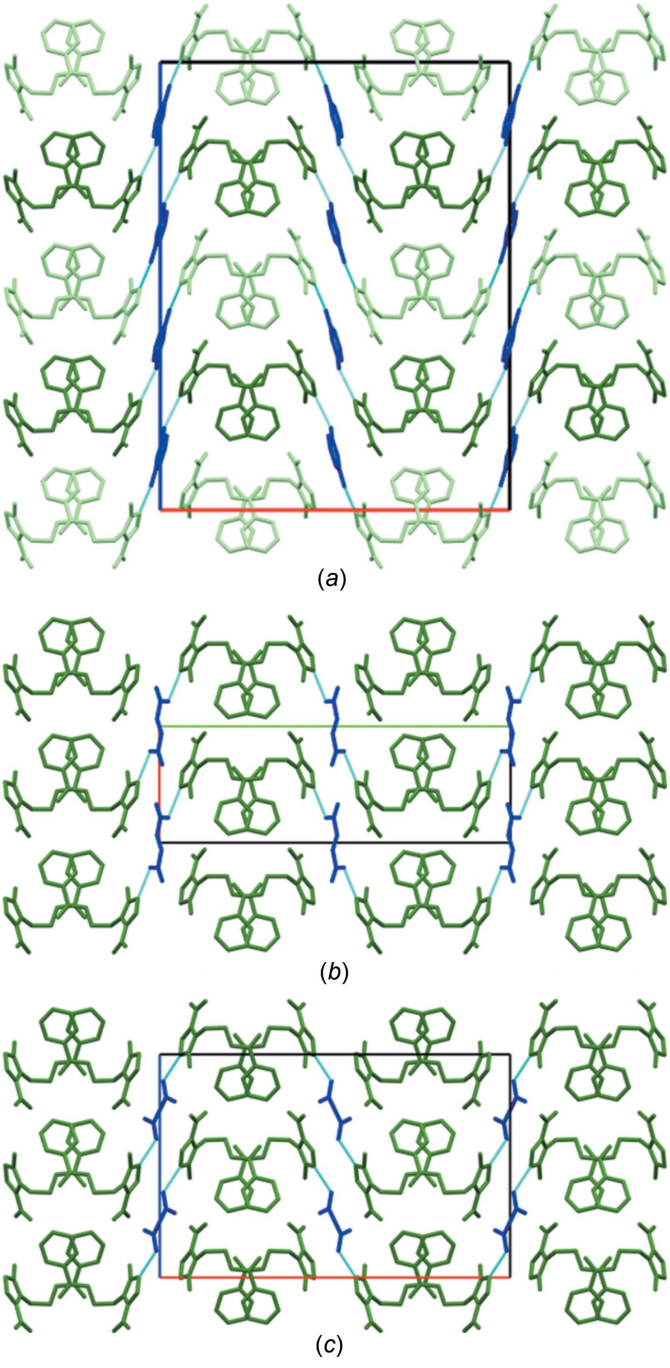


Figure 5
Projection of the crystal packing of (*a*) BZMDRES (*b* axis), (*b*) BZMDFMA (*c* axis) and (*c*) BZMDMLN (*c* axis). H atoms have been omitted for clarity. BZMD is represented in green and coformers in blue. Lattice axes *a*, *b* and *c* are colour-coded red, green and blue, respectively.

packing of intercalated columns observed in several of the reported structures (Fig. 5*a*).

After observing the hindrance of the second hydroxy group in MLC due to an intramolecular interaction, a natural coformer candidate is the *trans* isomer FMA. A BZMDFMA cocrystal was obtained with $Z' = 0.5$. This is because the FMA molecule lies on an inversion centre and half of it is in the asymmetric unit. As a consequence, the cocrystal stoichiometry is 2:1, as expected from our crystal-design strategy. Thus, the FMA coformer links two equivalent BZMD molecules by the proposed synthon [1.66 (4) Å], with the same crystal packing as observed in BZMDRES (Fig. 5*b*). The last coformer of this group is MLN, whose structure is similar to BZMDFMA. Also having $Z' = 0.5$, MLN lies in a twofold axis and is bonded to equivalent BZMD molecules by an Im···H—O interaction (1.9 and 2.3 Å), giving rise to the same crystal packing. Notice that the carboxylic acid group is disordered between two orientations and, as a consequence, the corresponding H atom cannot be unequivocally located from the difference maps. However, two facts support the classification of BZMDMLN as a cocrystal. First, no residual charges were observed near the N atom of the imidazole group. Furthermore, the C—O distances of both components of the disordered model have values which can be associated with a protonated carboxylic acid group, as will be discussed later.

3.1.3. Triple donor coformers. Considering the success of our crystal-design strategy to produce 2:1 cocrystals, the next step was to test coformers with three hydroxy groups in order to reach a 3:1 stoichiometry. Thus, new multicomponent forms were crystallized using 2,6DBA and 3,5DBA (Fig. 6).

BZMD2,6DBA (Fig. 6*a*) has three binding sites, but just one of them forms an intermolecular interaction involving the projected synthon. The remaining hydroxy groups are beside the carbonyl moiety and, as may be expected from the previous results, they form intramolecular hydrogen bonds

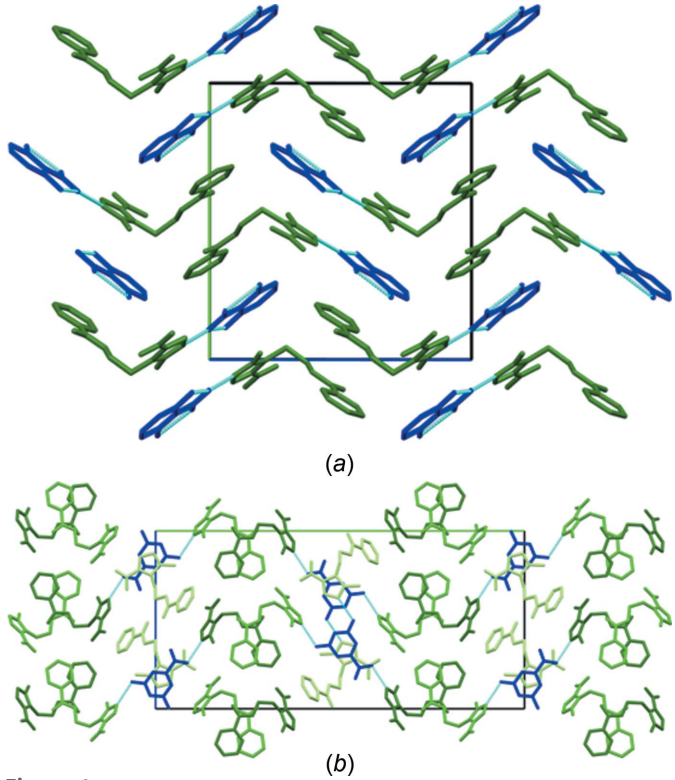


Figure 6
Packing of (*a*) the salt BZMD2,6DBA and (*b*) the cocrystal BZMD3,5DBA along the *a* axis. H atoms have been omitted for clarity. BZMD is represented in green and coformers in blue. Lattice axes *a*, *b* and *c* are colour-coded red, green and blue, respectively.

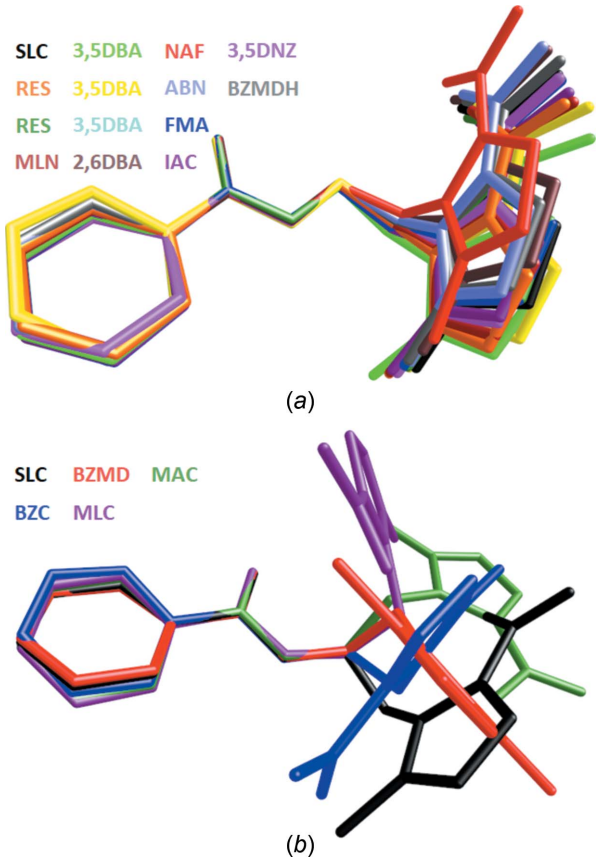


Figure 7
Comparison of the observed BZMD molecular conformations overlapping the ethyl groups and colour labelled based on the corresponding conformer. H atoms have been omitted for clarity.

blocking the Im···H—O interactions. Regarding the target synthon, the refined position places the H atom approximately at the middle [1.24 (5) Å] of the donor–acceptor distance [2.564 (2) Å], closer to the imidazole group. This configuration could be classified as a salt, but it will be discussed in detail later. The crystalline packing was based on the alternation between the coformer and API molecules in a zigzag pattern. Due to the greater affinity for intramolecular interactions in the coformer, the BZMD2,6DBA stoichiometry is 1:1, despite the availability of three binding sites.

According to our proposal, the asymmetric unit of BZMD3,5DBA (Fig. 6*b*) consists of three molecules of BZMD and one molecule of 3,5DBA, with the hydroxy groups actively participating in the proposed intermolecular hydrogen bonds, confirming a 3:1 stoichiometry based purely on the Im–HO synthon [1.73 (4), 1.78 (4) and 1.83 (4) Å]. The crystal packing resembles those of the 2:1 structures, but the third BZMD molecule is intercalated in the coformer column. The last coformer combines several of the key concepts addressed in our crystal-design strategy. First, the Im···H—O interaction is a reliable synthon for supramolecular structures, where the hydroxy group can be provided by molecules containing phenol and/or carboxylic acid groups. Several binding sites can be used to reach higher API–coformer stoichiometries, but intramolecular hydrogen bonds and/or

Table 2
Selected dihedral angles (°) of the BZMD molecule in single and multicomponent solid forms.

The θ column lists the angles between the planes defined by the imidazole (BZMD) and phenyl/carboxylic (coformer) groups.

		φ_1	φ_2	φ_3	φ_4	φ_5	θ
1	BZMD	104.1	−63.9	−94.9	178.6	−10.6	–
2	BZMDH	100.9	−66.4	−178.4	179.5	−6.3	–
3	SLC	111.0	−70.2	−170.8	177.4	7.3	3.8
4	3,5DBA	110.3	−67.7	−169.5	−168.7	−11.8	5.7
5	RES	106.6	−59.8	−174.0	−171.8	6.5	30.3
6	NAF	105.6	−68.8	170.5	178.3	9.0	6.9
7	3,5DBA	105.4	−63.4	−159.1	179.4	7.4/10.9	83.7
8	RES	105.1	−71.5	−169.1	175.6	3.7	31.6
9	3,5DBA	104.0	−63.6	−171.5	−178.6	17.8	89.9
10	ABN	103.6	−62.5	178.6	−179.1	−3.1	13.2
11	FMA	103.3	−70.5	−169.6	175.9	3.8	22.6
12	MLN	102.9	−61.5	−173.2	−172.9	7.5	22.8/29.3
13	2,6DBA	102.4	−73.5	−177.2	178.4	3.4	5.5
14	3,5DNZ	99.8	−65.5	−173.9	−178.0	20.2	75.4
15	IAC	99.8	−65.9	−168.4	177.1	4.4	20.4
16	MAC	94.5	−171.0	81.6	171.2	−10.4	5.1
17	BZC	−82.9	−63.0	159.2	−178.2	−11.0	17.5
18	MLC	−72.7	−66.7	98.1	170.2	−14.7	59.9

coformer dimers could limit the available coformers. The first problem can be addressed by selecting appropriate molecular structures, whereas the competition between coformer homosynthons and Im···H—O interactions should be solved by serendipity.

4. Discussion

After presenting several new solid forms of BZMD, it is interesting to perform a comparative analysis between these structures. As a starting point, the molecular conformation of the API molecule will be considered. Comparing the observed BZMD molecular conformations (Fig. 7), it may be concluded that the main changes are related to the orientation among the phenyl, ethyl formate and imidazole groups. Table 2 lists the backbone dihedral angles of the BZMD molecule for all the structures reported in this contribution following the notation of Fig. 1. By overlapping the ethyl formate groups, it is possible to notice that the structures differ mainly by rotations of the imidazole and phenyl moieties. In particular, the phenyl group is always slightly out of the plane of the ethyl formate chain ($|\varphi_5| < 20°$). This conformational flexibility does not seem to be determinant for the crystal packing, but a mechanism to optimize API–API interactions in the BZMD columns (see, for example, Fig. 5). Considering the imidazole group and following the numbering of Table 2, the set of crystalline structures **3** to **15** (Fig. 7*a*) exhibit a continuous change in the dihedral angle associated with the orientation of this moiety (φ_1). Notice that BZMDH can be included in this set but not BZMD, showing that this conformation is favourable for the crystal packing of multicomponent forms. The largest dihedral angle associated with the orientation of the imidazole ring (φ_1) corresponds to BZMDSLC (111°) and the smallest to BZMDIAC (99.8°). It is also interesting to observe that all the non-equivalent molecules of the higher stoichio-

metry forms (BZMDRES and BZMD3,5DBA) lie between these limits. Finally, BZMD and three cocrystals (**16**, **17** and **18**) differ considerably from the previous set and need to be considered separately, as shown in Fig. 7(*b*), where BZMDSLC (**3**) was included as a reference. The characteristic feature of this set is the flipping of the methylnitroimidazole group compared with BZMDSLC. Besides that, they have larger rotations of the imidazole group, which also induce additional torsion in the ethyl formate chain (φ_2 and φ_3).

The conformational changes of the BZMD molecules are directly related to the backbone of the supramolecular structure defined by the API. In the *Results* (§3) section, several structures have been described as being formed by BZMD columns/layers with intercalated coformers. The key interaction in this packing is the π-stacking of the BZMD molecules (see Table S3 in the supporting information). Two kinds of π–π interactions between BZMD molecules were observed in cocrystal/salts, *i.e.* imidazole–phenyl and phenyl–phenyl, and only BZMDH exhibits an imidazole–imidazole interaction. Despite the involved rings, all the π–π interactions can be classified as approximately parallel ($\alpha < 20^\circ$), but not face-centred (offset > 1.3 Å) (Martinez & Iverson, 2012). Representative interactions are shown in Fig. 8 evidenced by the BZMD Hirshfeld surface mapped with the shape index, which exhibits a 'bow-tie' pattern of red–blue triangles fingerprinting the π–π interactions (McKinnon *et al.*, 2004; Spackman & Jayatilaka, 2009). Imidazole–phenyl interactions are observed with the BZC, MAC and DNZ coformers (Fig. 2), but, in BZMDBZC and BZMDMAC, the API forms dimers intercalated with the coformers. The π-stacked columns are present in BZMD3,5DNZ, which resemble the columns in Fig. 5 defined by phenyl–phenyl interactions. In fact, the stacking of the phenyl rings is the most prevalent backbone in the BZMD multicomponent forms, being observed with the coformers SLC, MLC, IAC (Fig. 4), RES, FMA, MLN (Fig. 5) and 3,5DBA (Fig. 6). The π-stacking is also evident in the alternative projection shown in Fig. 4 for MLC and IAC. In the remaining structures, *i.e.* BZMDABN, BZMDNAF and BZMD2,6DBA, the aromatic rings of the coformers determine the supramolecular organization by API–coformer interactions. These kinds of interactions are also observed in several of the previously described structures, but the API–API interaction plays a key role in the crystal packing (see Table S3 in the supporting information). It is also interesting to notice that the molecular conformation shown in Fig. 7(*a*) really favours the π-stacking and, consequently, multicomponent BZMD forms.

Regarding the API–coformer Im–HO synthon, the first point to be considered is the charge transfer between these molecules. According to the pK_a rule, based on the probability of proton transfer between the components in a reaction, the pK_a difference [ΔpK_a = pK_a(protonated base) − pK_a(acid)] can be used as a predictor of the formation of a cocrystal/salt (Delori *et al.*, 2013). Based on a detailed statistical analysis, Cruz-Cabeza (2012) identified three types of behaviour: (i) where cocrystals are almost exclusively formed ($\Delta K_a < -1$), (ii) where salts are prevalent ($\Delta K_a > 4$) and (iii) a co-existence region where both salts and cocrystals can be observed ($-1 \leq \Delta K_a \leq 4$). In the co-existence region, complex proton behaviours can be observed not allowing the classification of those structures under one of the proton-transfer conditions, giving rise to the 'salt–cocrystal continuum' (Childs *et al.*, 2011; da Silva *et al.*, 2013). In good agreement with this rule, nine of the conformers give rise to cocrystals, once the difference between the pK_a of the drug and coformer is lower than −1 (see Table S4 in the supporting information). The remaining API–coformer pairs are in the co-existence region, with most of them having Δp$K_a < 0$ and being identified as cocrystals. Two cases need to be considered separately, BZMDMLC (ΔpK_a = 0.72) and BZMD2,6DBA (ΔpK_a = −0.22), because the corresponding crystalline structures cannot be described as cocrystals. In the case of BZMDMLC, the proton was located and refined based on the difference Fourier maps, placing it close to the imidazole group characterizing a salt. Considering the linear relationship established by Cruz-Cabeza (2012), the BZMD/MLC pair has a probability of 40.2% of crystallizing as a salt. On the other hand, in the BZMD/2,6DBA system, this probability is 24.3%, which is also the highest probability observed among the BZMD cocrystals reported here. The

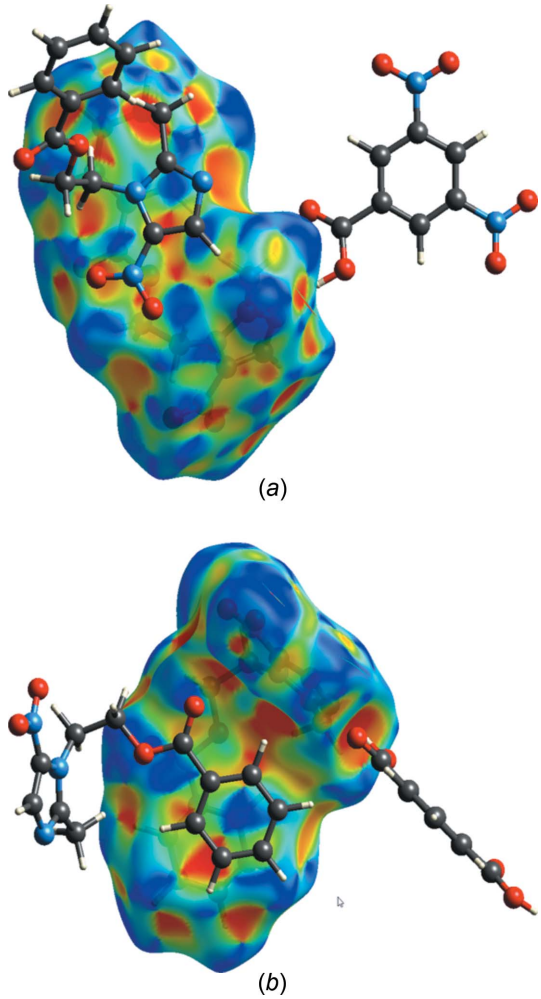


Figure 8
Hirshfeld surfaces mapped with the shape index of (*a*) BZMDBZC and (*b*) BZMDIAC, showing the π-stacking of the BZMD columns.

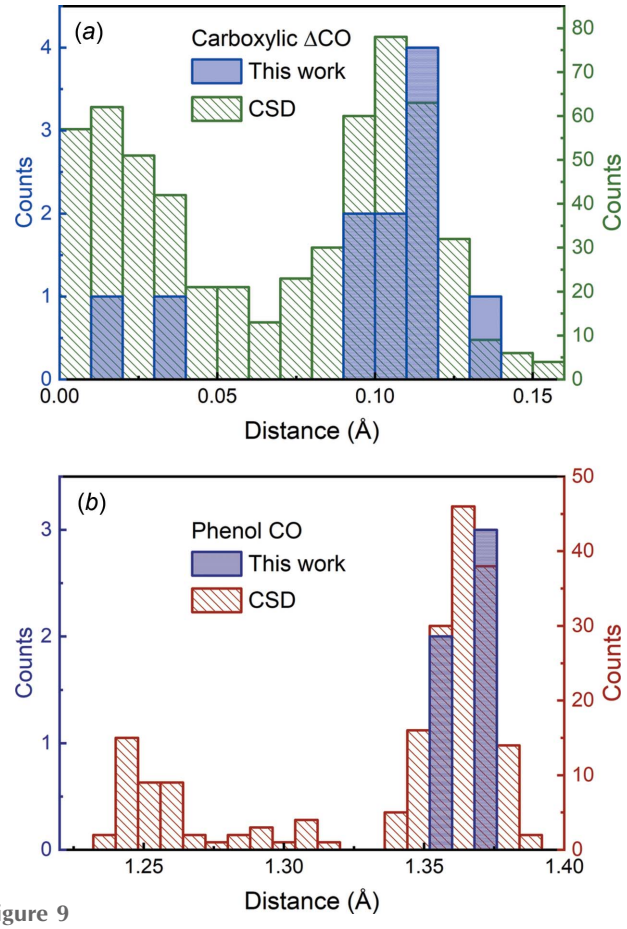


Figure 9
(*a*) Distribution of the difference between the C—O distances of the carboxylic acid group. (*b*) Distribution of the C—O distances of the phenol groups.

proton position refinement placed it slightly closer to the imidazole group, but with the largest donor–hydrogen distance (1.24 Å). Even though several of the structures reported here could be predicted based on the ΔpK_a rule, from the point of view of the proper classification of multicomponent forms as cocrystals or salts, other markers can be used. Based on the proposed synthon, the determined structures were compared with a search performed in the CSD for the Im–carboxylic and Im–phenol synthons. The hits related to carboxylic acid were processed calculating the difference (ΔCO) between the two C—O bond lengths. It is well known that a ΔCO lower than ∼0.03 Å indicates that the carboxylic acid group is deprotonated. The analysis of the Im–carboxylic acid hits agrees with this rule as two distributions are observed (Fig. 9*a*), which are centred around ΔCO = ∼0.105 and ∼0.0 Å, being related to protonated and deprotonated carboxylic acid groups, respectively. Comparing this distribution with the BZMD salts/cocrystals, one may conclude that all the ΔCO cocrystals lie in the expected region. In the case of the salts, the lowest hit (ΔCO = 0.016 Å) corresponds to BZMDMLC, which is in good agreement with the salt character predicted by the ΔpK_a rule. Just above this hit, there is that from BZMD2,6DBA (ΔCO = 0.0354 Å), which is in the co-existence region of the ΔpK_a rule, but lies around the upper limit of the deprotonated region in the ΔCO plot, confirming that this multicomponent form was correctly classified as a salt. For the case of the Im–phenol synthon, the statistical distribution of C—O distances is shown in Fig. 9(*b*). These distances are mainly distributed around two maxima at 1.25 and 1.36 Å, which are related to deprotonated and protonated hydroxy groups, respectively. As expected, the C—O distances of the BZMD cocrystals based on phenols are in the range of the protonated hydroxy distances, confirming the previous classification.

The previous results clearly confirm the reliability of the Im–carboxylic and Im–phenol synthons as a crystal-design strategy to produce multicomponent forms with variable stoichiometry. Comparing the crystalline structures, three synthon geometries were identified and the Im–phenol synthon was observed with the coformers RES, NAF and 3,5DBA. On the other hand, the simple Im–carboxylic acid synthon, with and without charge transfer, is present in forms containing ABN, IAC, FMA, MLC, MLN, SLC, 2,6DBA and 3,5DNZ. A third synthon derived from Im–carboxylic acid forms an $R_2^2(8)$ ring including the methyl moiety of the methylnitroimidazole group. BZC and MAC use the last synthon to stabilize their crystalline structures. These synthons can also be analyzed by comparing the acceptor–donor distances of the structures reported in this work with those in

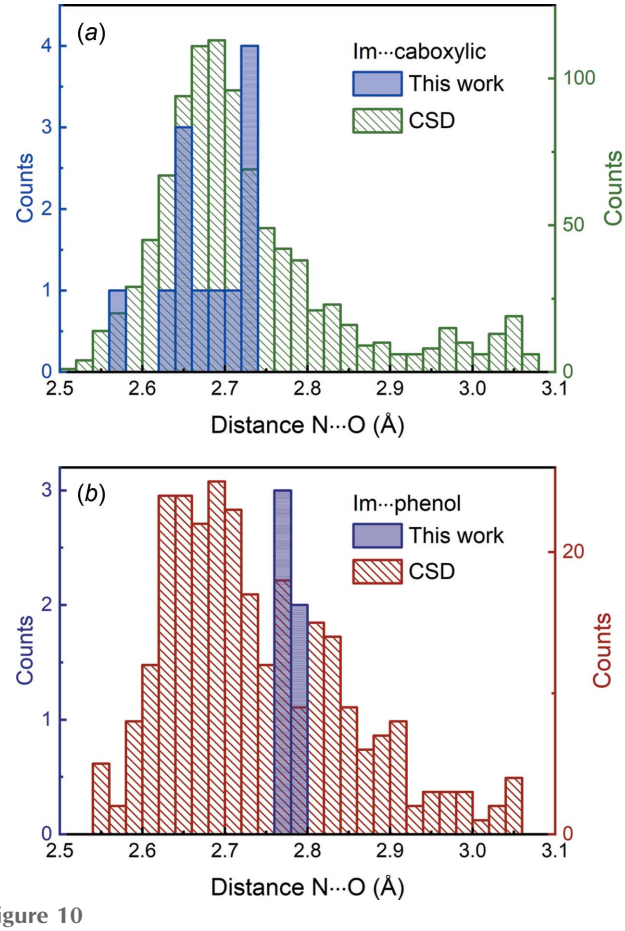


Figure 10
Comparison of the distribution of the acceptor–donor distances of the synthons based on (*a*) carboxylic acid and (*b*) phenol groups.

the CSD. Fig. 10 shows the histograms of the N—O distances when carboxylic acid or phenol groups are considered. Both synthons have well-defined distributions spanning approximately the same value range, with that related to the phenol group being a little wider. The acceptor–donor distances calculated from the BZMD new forms lie within the general distribution ranges, despite the fact that the phenol-based cocrystals exhibit distances slightly longer than the distribution maxima. Another interesting parameter is the angle (θ) between the plane containing the imidazole ring and either that defined by the phenyl or the carboxylic acid group. Despite which synthon is used, there is no clear relationship among the angles listed in Table 2, showing that the proposed synthon does not restrict the relative orientation of the API and coformer, giving the new forms plenty of flexibility to optimize the supramolecular organization.

5. Conclusion

This work was aimed at rationally designing multicomponent forms of BZMD. To achieve this goal, a target supramolecular synthon was selected on the basis of the BZMD molecular structure and a statistical analysis of the Cambridge Structural Database. Thus, the imidazole group of BZMD seems to be a suitable acceptor for hydrogen bonds with coformers containing hydroxy groups. In order to explore different stoichiometries from the same synthon (1:1, 2:1 and 3:1), we choose coformers with carboxylic acid and phenol groups, based on the available binding sites. This strategy generated thirteen new solid forms (two salts and eleven cocrystals). At first, coformers with a single hydroxy donor (BZC, NAF, MAC, 3,5DNZ and ABN) were selected and multicomponent structures with a 1:1 stoichiometry were produced, proving that the proposed strategy was successful. Coformers containing two binding sites were tested in order to explore solid forms with a 2:1 stoichiometry. In this sense, carboxylic acids and phenols with donor groups were selected, but despite the fact that these coformers have two hydroxy groups, several of them crystallize with a 1:1 stoichiometry. It was observed that two effects could limit synthon formation. In coformers with close hydroxy groups (SLC and MLC), intramolecular hydrogen bonds are more favourable than the Im–HO synthon. Furthermore, coformer homosynthons (IAC) could also reduce the number of active sites available to be linked to the API. Based on these observations, the molecular geometry of the coformer was chosen in order to avoid intramolecular hydrogen bonds and three cocrystals with a 2:1 stoichiometry were produced (RES, FMA and MLN). The next step was to test coformers with three hydroxy groups in order to reach a 3:1 stoichiometry. Thus, new multicomponent forms were crystallized using 2,6DBA and 3,5DBA. The former has intramolecular hydrogen bonds limiting the stoichiometry to 1:1, but a 3:1 ratio was achieved with 3,5DBA, combining carboxylic and phenol synthons. When compared with other hits in the CSD, the intermolecular parameters of the Im–HO synthon in the BZMD cocrystals/salts are similar, showing that this is a robust synthon. In addition, the lack of a geometrical constraint in the relative orientation of the API and coformer provides additional flexibility to the selected interaction, confirming that Im–HO is a trustworthy synthon for use in a crystal-design strategy.

Funding information

Funding for this research was provided in part by: the Brazilian agencies CAPES (Finance Code 001), FUNCAP (PPSUS and PRONEX PR2-0101-00006.01.00/15), and CNPq.

References

Aitipamula, S., Chow, P. S. & Tan, R. B. H. (2014). *CrystEngComm*, **16**, 3451–3465.
Babu, N. J., Sanphui, P. & Nangia, A. (2012). *Chem. Asian J.* **7**, 2274–2285.
Barikah, K. Z. (2018). *Syst. Rev. Pharm.* **9**, 79–82.
Bempong, D. K., Manning, R. G., Mirza, T. & Bhattacharyya, L. (2005). *J. Pharm. Biomed. Anal.* **38**, 776–780.
Berry, D. J. & Steed, J. W. (2017). *Adv. Drug Deliv. Rev.* **117**, 3–24.
Blagden, N., de Matas, M., Gavan, P. T. & York, P. (2007). *Adv. Drug Deliv. Rev.* **59**, 617–630.
Bolla, G. & Nangia, A. (2016). *Chem. Commun.* **52**, 8342–8360.
Bruker (2012). *APEX3*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2016). *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Caira, M. R., Nassimbeni, L. R. & van Oudtshoorn, B. (1993). *J. Pharm. Sci.* **82**, 1006–1009.
Cerreia Vioglio, P., Chierotti, M. R. & Gobetto, R. (2017). *Adv. Drug Deliv. Rev.* **117**, 86–110.
Childs, S. L., Stahly, G. P. & Park, A. (2011). *Mol. Pharm.* **4**, 323–338.
Corpinot, M. K. & Bučar, D.-K. (2018). *Cryst. Growth Des.* **19**, 1426–1453.
Cruz-Cabeza, A. J. (2012). *CrystEngComm*, **14**, 6362–6365.
Dalpiaz, A., Pavan, B. & Ferretti, V. (2017). *Drug Discov. Today*, **22**, 1134–1138.
Delori, A., Friščić, T. & Jones, W. (2012). *CrystEngComm*, **14**, 2350–2362.
Delori, A., Galek, P. T. A., Pidcock, E., Patni, M. & Jones, W. (2013). *CrystEngComm*, **15**, 2916–2928.
Desiraju, G. R. (2010). *J. Chem. Sci.* **122**, 667–675.
Diniz, L. F., Souza, M. S., Carvalho, P. S. Jr, da Silva, C. C. P., D'Vries, R. F. & Ellena, J. (2018). *J. Mol. Struct.* **1153**, 58–68.
Do, J. L. & Friscic, T. (2017). *ACS Cent. Sci.* **3**, 13–19.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Douroumis, D., Ross, S. A. & Nokhodchi, A. (2017). *Adv. Drug Deliv. Rev.* **117**, 178–195.
EMA (2015). *Reflection Paper on the Use of Cocrystals of Active Substances in Medicinal Products*. https://www.ema.europa.eu/en/.
FDA (2018). *Guidance for Industry – Regulatory Classification of Pharmaceutical Cocrystals*. https://www.fda.gov/.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hasa, D. & Jones, W. (2017). *Adv. Drug Deliv. Rev.* **117**, 147–161.
Healy, A. M., Worku, Z. A., Kumar, D. & Madi, A. M. (2017). *Adv. Drug Deliv. Rev.* **117**, 25–46.
Hoelgaard, A. & Møller, N. (1983). *Int. J. Pharm.* **15**, 213–221.
James, S. L., Adams, C. J., Bolm, C., Braga, D., Collier, P., Friščić, T., Grepioni, F., Harris, K. D., Hyett, G., Jones, W., Krebs, A., Mack, J., Maini, L., Orpen, A. G., Parkin, I. P., Shearouse, W. C., Steed, J. W. & Waddell, D. C. (2012). *Chem. Soc. Rev.* **41**, 413–447.
Kavanagh, O. N., Croker, D. M., Walker, G. M. & Zaworotko, M. J. (2019). *Drug Discov. Today*, **24**, 796–804.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Martinez, C. R. & Iverson, B. L. (2012). *Chem. Sci.* **3**, 2191–2201.
McKinnon, J. J., Spackman, M. A. & Mitchell, A. S. (2004). *Acta Cryst.* B**60**, 627–668.
Pedretti, A., Villa, L. & Vistoli, G. (2004). *J. Comput. Aided Mol. Des.* **18**, 167–173.
Peraka, K. S., Lusi, M., Bajpai, A. & Zaworotko, M. J. (2017). *Cryst. Growth Des.* **17**, 959–962.
Saha, S. & Desiraju, G. R. (2018). *J. Am. Chem. Soc.* **140**, 6361–6373.
Sarkar, A. & Rohani, S. (2015). *J. Pharm. Sci.* **104**, 98–105.
Sarraguça, M. C., Paisana, M., Pinto, J. & Lopes, J. A. (2016). *Eur. J. Pharm. Sci.* **90**, 76–84.
Shaikh, R., Singh, R., Walker, G. M. & Croker, D. M. (2018). *Trends Pharmacol. Sci.* **39**, 1033–1048.
Shayanfar, A. & Jouyban, A. (2014). *Powder Technol.* **262**, 242–248.
Shayanfar, A., Velaga, S. & Jouyban, A. (2014). *Fluid Phase Equilib.* **363**, 97–105.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Silva, C. C. P. da, de Oliveira, R., Tenorio, J. C., Honorato, S. B., Ayala, A. P. & Ellena, J. (2013). *Cryst. Growth Des.* **13**, 4315–4322.
Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Spek, A. L. (2015). *Acta Cryst.* C**71**, 9–18.
Wang, T., Stevens, J. S., Vetter, T., Whitehead, G. F. S., Vitorica-Yrezabal, I. J., Hao, H. & Cruz-Cabeza, A. J. (2018). *Cryst. Growth Des.* **18**, 6973–6983.

supporting information

Acta Cryst. (2019). C**75**, 483-495 [https://doi.org/10.1107/S2053229619003838]

The design of novel metronidazole benzoate structures: exploring stoichiometric diversity

Yara Santiago de Oliveira, Wendell Saraiva Costa, Poliana Ferreira Borges, Maria Silmara Alves de Santana and Alejandro Pedro Ayala

Computing details

For all structures, data collection: *APEX3* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009), *Mercury* (Version 3.10; Macrae *et al.*, 2008) and *VEGA* (Pedretti *et al.*, 2004); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–benzoic acid (1/1) (bzmdbzc)

Crystal data

$C_{13}H_{13}N_3O_4{\cdot}C_7H_6O_2$
M_r = 397.38
Monoclinic, $P2_1/n$
a = 13.5997 (6) Å
b = 9.0354 (4) Å
c = 16.5974 (8) Å
β = 108.646 (2)°
V = 1932.42 (15) Å^3
Z = 4
$F(000)$ = 832
D_x = 1.366 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9997 reflections
θ = 5.1–68.0°
μ = 0.86 mm^{-1}
T = 300 K
Prism, clear light colourless
0.8 × 0.2 × 0.2 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.675, T_{max} = 0.753
60527 measured reflections
3542 independent reflections
2669 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 68.3°, θ_{min} = 3.7°
h = −16→16
k = −10→10
l = −19→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.130
S = 1.07
3542 reflections
339 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.7992P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0027 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.57161 (11)	0.97707 (18)	0.14818 (9)	0.0723 (4)
O1′	0.65654 (13)	0.60123 (18)	0.53629 (11)	0.0806 (5)
N1	0.62802 (12)	0.99073 (17)	0.32969 (9)	0.0568 (4)
O2′	0.52139 (13)	0.69513 (19)	0.56528 (12)	0.0887 (5)
N3	0.79953 (14)	0.9851 (2)	0.30460 (11)	0.0681 (5)
O1	0.87927 (13)	0.9118 (2)	0.31765 (12)	0.0933 (5)
N2	0.65260 (13)	0.80491 (19)	0.42084 (11)	0.0655 (5)
O4	0.43536 (12)	0.8503 (2)	0.06689 (11)	0.0930 (6)
O2	0.78341 (14)	1.1005 (2)	0.26413 (12)	0.0933 (6)
C1′	0.61614 (14)	0.4999 (2)	0.65137 (12)	0.0543 (4)
C1	0.72512 (15)	0.9308 (2)	0.34107 (12)	0.0584 (5)
C8	0.60097 (15)	0.8057 (2)	0.05160 (12)	0.0605 (5)
C7′	0.59173 (15)	0.6076 (2)	0.57987 (12)	0.0587 (5)
C3	0.58695 (16)	0.9091 (2)	0.37957 (12)	0.0587 (5)
C6′	0.54581 (18)	0.4792 (2)	0.69523 (14)	0.0660 (5)
C2′	0.70976 (16)	0.4248 (2)	0.67683 (15)	0.0670 (5)
C7	0.52666 (16)	0.8765 (3)	0.08774 (12)	0.0642 (5)
C2	0.73912 (17)	0.8177 (2)	0.39708 (14)	0.0660 (5)
C5	0.5730 (2)	1.1090 (2)	0.27249 (15)	0.0692 (6)
C9	0.5671 (2)	0.6840 (3)	−0.00055 (15)	0.0765 (6)
C4	0.4827 (2)	0.9323 (3)	0.38706 (18)	0.0732 (6)
C6	0.50507 (19)	1.0484 (3)	0.18877 (14)	0.0755 (6)
C5′	0.5698 (2)	0.3854 (3)	0.76467 (15)	0.0746 (6)
C13	0.70145 (18)	0.8566 (3)	0.06717 (15)	0.0725 (6)
C4′	0.6644 (2)	0.3150 (3)	0.79135 (16)	0.0786 (7)
C12	0.7663 (2)	0.7852 (3)	0.03012 (18)	0.0836 (7)
C11	0.7312 (2)	0.6645 (3)	−0.02131 (17)	0.0872 (8)
C3′	0.7339 (2)	0.3331 (3)	0.74715 (17)	0.0807 (7)

C10	0.6321 (2)	0.6133 (3)	−0.03665 (18)	0.0900 (8)
H9	0.497 (2)	0.656 (3)	−0.0102 (16)	0.086 (7)*
H12	0.838 (2)	0.821 (3)	0.0425 (18)	0.107 (9)*
H11	0.774 (2)	0.614 (3)	−0.0500 (16)	0.095 (8)*
H2′	0.7584 (18)	0.435 (3)	0.6439 (14)	0.080 (7)*
H4′	0.679 (2)	0.249 (3)	0.8403 (18)	0.105 (9)*
H6′	0.477 (2)	0.532 (3)	0.6729 (15)	0.092 (8)*
H5′	0.520 (2)	0.375 (3)	0.7942 (16)	0.094 (8)*
H3′	0.801 (2)	0.276 (3)	0.7636 (18)	0.111 (9)*
H13	0.7269 (19)	0.943 (3)	0.1044 (16)	0.087 (8)*
H2	0.8006 (19)	0.756 (3)	0.4194 (15)	0.083 (7)*
H6A	0.450 (2)	0.972 (3)	0.1934 (17)	0.101 (9)*
H6B	0.468 (2)	1.128 (3)	0.1501 (17)	0.098 (8)*
H1′	0.647 (2)	0.681 (4)	0.494 (2)	0.138 (12)*
H5A	0.6277 (18)	1.174 (3)	0.2639 (15)	0.081 (7)*
H5B	0.5303 (18)	1.163 (3)	0.3013 (15)	0.079 (7)*
H4A	0.474 (2)	0.864 (3)	0.4331 (19)	0.110 (9)*
H4B	0.428 (2)	0.917 (3)	0.336 (2)	0.109 (10)*
H4C	0.476 (2)	1.031 (4)	0.4081 (17)	0.102 (9)*
H10	0.608 (2)	0.526 (4)	−0.072 (2)	0.123 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0652 (9)	0.0906 (11)	0.0624 (8)	−0.0003 (8)	0.0223 (7)	−0.0020 (8)
O1′	0.0944 (11)	0.0741 (10)	0.0880 (11)	0.0183 (8)	0.0497 (9)	0.0230 (9)
N1	0.0661 (10)	0.0539 (9)	0.0508 (8)	0.0004 (7)	0.0194 (7)	0.0009 (7)
O2′	0.0776 (10)	0.0867 (12)	0.1086 (13)	0.0266 (9)	0.0395 (9)	0.0356 (10)
N3	0.0712 (11)	0.0709 (11)	0.0642 (10)	−0.0079 (9)	0.0246 (9)	−0.0045 (9)
O1	0.0775 (11)	0.0989 (13)	0.1149 (14)	0.0056 (10)	0.0466 (10)	0.0036 (11)
N2	0.0694 (10)	0.0638 (10)	0.0634 (10)	−0.0010 (8)	0.0213 (8)	0.0078 (8)
O4	0.0621 (9)	0.1282 (15)	0.0868 (11)	−0.0115 (10)	0.0211 (8)	−0.0059 (11)
O2	0.0977 (12)	0.0898 (12)	0.0998 (13)	−0.0056 (10)	0.0421 (10)	0.0267 (10)
C1′	0.0576 (10)	0.0471 (10)	0.0568 (10)	−0.0020 (8)	0.0164 (8)	−0.0019 (8)
C1	0.0622 (11)	0.0585 (11)	0.0560 (11)	−0.0049 (9)	0.0211 (9)	−0.0028 (9)
C8	0.0641 (11)	0.0678 (12)	0.0490 (10)	−0.0042 (9)	0.0171 (9)	0.0126 (9)
C7′	0.0580 (11)	0.0538 (11)	0.0630 (12)	−0.0023 (9)	0.0173 (9)	0.0011 (9)
C3	0.0682 (12)	0.0574 (11)	0.0519 (10)	−0.0038 (9)	0.0211 (9)	−0.0028 (9)
C6′	0.0706 (13)	0.0630 (12)	0.0693 (13)	0.0057 (10)	0.0293 (11)	0.0018 (10)
C2′	0.0599 (12)	0.0633 (12)	0.0773 (14)	0.0022 (10)	0.0211 (10)	0.0091 (10)
C7	0.0631 (12)	0.0762 (14)	0.0506 (11)	−0.0043 (10)	0.0144 (9)	0.0122 (10)
C2	0.0655 (12)	0.0642 (12)	0.0668 (13)	0.0012 (10)	0.0192 (10)	0.0044 (10)
C5	0.0848 (15)	0.0568 (12)	0.0707 (14)	0.0127 (11)	0.0315 (12)	0.0103 (10)
C9	0.0744 (15)	0.0848 (16)	0.0674 (13)	−0.0092 (13)	0.0188 (11)	0.0021 (12)
C4	0.0734 (14)	0.0808 (16)	0.0712 (15)	0.0014 (12)	0.0311 (12)	0.0003 (13)
C6	0.0740 (14)	0.0941 (17)	0.0592 (12)	0.0181 (13)	0.0223 (11)	0.0103 (12)
C5′	0.0915 (16)	0.0737 (14)	0.0683 (13)	0.0026 (12)	0.0394 (13)	0.0054 (11)
C13	0.0696 (13)	0.0772 (15)	0.0733 (14)	−0.0081 (12)	0.0263 (11)	0.0079 (12)

C4′	0.0926 (17)	0.0731 (15)	0.0672 (14)	0.0018 (13)	0.0215 (12)	0.0134 (12)
C12	0.0728 (15)	0.0937 (19)	0.0905 (17)	−0.0004 (13)	0.0351 (13)	0.0171 (15)
C11	0.100 (2)	0.0925 (19)	0.0790 (16)	0.0190 (16)	0.0419 (15)	0.0129 (14)
C3′	0.0693 (14)	0.0779 (15)	0.0886 (16)	0.0102 (12)	0.0165 (12)	0.0210 (13)
C10	0.100 (2)	0.0892 (19)	0.0812 (17)	0.0005 (16)	0.0299 (15)	−0.0058 (14)

Geometric parameters (Å, º)

O3—C7	1.347 (3)	C1′—C2′	1.384 (3)
O3—C6	1.441 (3)	C1—C2	1.353 (3)
O1′—C7′	1.308 (2)	C8—C7	1.476 (3)
N1—C1	1.383 (2)	C8—C9	1.384 (3)
N1—C3	1.355 (2)	C8—C13	1.386 (3)
N1—C5	1.466 (3)	C3—C4	1.477 (3)
O2′—C7′	1.205 (2)	C6′—C5′	1.383 (3)
N3—O1	1.230 (2)	C2′—C3′	1.382 (3)
N3—O2	1.221 (2)	C5—C6	1.504 (3)
N3—C1	1.422 (3)	C9—C10	1.374 (4)
N2—C3	1.327 (3)	C5′—C4′	1.376 (3)
N2—C2	1.360 (3)	C13—C12	1.385 (4)
O4—C7	1.201 (2)	C4′—C3′	1.379 (4)
C1′—C7′	1.488 (3)	C12—C11	1.373 (4)
C1′—C6′	1.387 (3)	C11—C10	1.370 (4)
C7—O3—C6	116.51 (17)	N1—C3—C4	124.6 (2)
C1—N1—C5	129.89 (17)	N2—C3—N1	111.14 (17)
C3—N1—C1	105.40 (16)	N2—C3—C4	124.22 (19)
C3—N1—C5	124.57 (18)	C5′—C6′—C1′	120.1 (2)
O1—N3—C1	116.53 (19)	C3′—C2′—C1′	119.9 (2)
O2—N3—O1	123.4 (2)	O3—C7—C8	112.86 (17)
O2—N3—C1	120.10 (19)	O4—C7—O3	121.9 (2)
C3—N2—C2	106.95 (17)	O4—C7—C8	125.2 (2)
C6′—C1′—C7′	119.43 (18)	C1—C2—N2	108.58 (19)
C2′—C1′—C7′	120.86 (18)	N1—C5—C6	111.62 (19)
C2′—C1′—C6′	119.65 (19)	C10—C9—C8	120.7 (2)
N1—C1—N3	125.81 (18)	O3—C6—C5	107.62 (19)
C2—C1—N1	107.93 (18)	C4′—C5′—C6′	119.9 (2)
C2—C1—N3	126.15 (19)	C12—C13—C8	119.5 (3)
C9—C8—C7	117.7 (2)	C5′—C4′—C3′	120.2 (2)
C9—C8—C13	119.5 (2)	C11—C12—C13	120.1 (3)
C13—C8—C7	122.9 (2)	C10—C11—C12	120.6 (3)
O1′—C7′—C1′	113.23 (17)	C4′—C3′—C2′	120.2 (2)
O2′—C7′—O1′	123.35 (19)	C11—C10—C9	119.6 (3)
O2′—C7′—C1′	123.38 (19)		

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–*β*-naphthol (1/1) (bzmdnaf)

Crystal data

$C_{13}H_{13}N_3O_4 \cdot C_{10}H_8O$
$M_r = 419.43$
Monoclinic, $P2_1/c$
$a = 8.5105$ (8) Å
$b = 22.387$ (2) Å
$c = 11.7752$ (11) Å
$\beta = 108.664$ (4)°
$V = 2125.4$ (3) Å^3
$Z = 4$
$F(000) = 880$
$D_x = 1.311$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 9803 reflections
$\theta = 4.4$–$69.6°$
$\mu = 0.78$ mm^{-1}
$T = 300$ K
Prism, clear light yellow
0.42 × 0.09 × 0.07 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.678$, $T_{max} = 1.000$
39131 measured reflections
3884 independent reflections
2810 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 68.3°$, $\theta_{min} = 4.0°$
$h = -10 \rightarrow 10$
$k = -26 \rightarrow 26$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.193$
$S = 1.06$
3884 reflections
365 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1113P)^2 + 0.4215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0041 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source ($\lambda = 0.71073$ Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	−0.36072 (19)	0.49428 (7)	0.19944 (13)	0.0624 (4)

O2	−0.2808 (2)	0.51266 (9)	0.57654 (16)	0.0842 (6)
N1	−0.2220 (2)	0.58230 (8)	0.39335 (15)	0.0563 (4)
O1	−0.0234 (3)	0.52273 (9)	0.68439 (16)	0.0850 (6)
O1′	0.2411 (3)	0.70227 (10)	0.35022 (19)	0.0908 (6)
N3	−0.1417 (3)	0.53251 (9)	0.59314 (17)	0.0652 (5)
O4	−0.3769 (3)	0.39564 (9)	0.21856 (18)	0.0892 (6)
N2	0.0181 (2)	0.62642 (9)	0.40900 (18)	0.0681 (5)
C1	−0.1092 (3)	0.56838 (9)	0.50416 (18)	0.0562 (5)
C3	−0.1374 (3)	0.61722 (10)	0.3393 (2)	0.0634 (6)
C8	−0.2958 (3)	0.43345 (12)	0.05661 (19)	0.0658 (6)
C2	0.0348 (3)	0.59617 (11)	0.5115 (2)	0.0649 (6)
C7	−0.3486 (3)	0.43791 (11)	0.1652 (2)	0.0633 (6)
C10′	0.4667 (3)	0.67583 (11)	0.5266 (2)	0.0675 (6)
C5	−0.3963 (3)	0.56412 (11)	0.3424 (2)	0.0645 (6)
C9′	0.6381 (3)	0.67996 (10)	0.5925 (2)	0.0688 (6)
C1′	0.4025 (3)	0.70428 (11)	0.4195 (2)	0.0727 (7)
C6	−0.4166 (3)	0.50046 (11)	0.3028 (2)	0.0623 (6)
C9	−0.2418 (3)	0.48176 (15)	0.0078 (2)	0.0772 (7)
C4′	0.7415 (3)	0.71446 (11)	0.5461 (3)	0.0799 (8)
C4	−0.2096 (5)	0.64272 (17)	0.2172 (3)	0.0859 (8)
C13	−0.2986 (4)	0.37744 (15)	0.0059 (2)	0.0836 (8)
C8′	0.7088 (4)	0.65030 (14)	0.7035 (3)	0.0846 (8)
C2′	0.5090 (5)	0.73895 (14)	0.3747 (4)	0.0921 (9)
C3′	0.6720 (4)	0.74335 (14)	0.4367 (4)	0.0989 (11)
C12	−0.2455 (5)	0.37083 (19)	−0.0939 (3)	0.0984 (10)
C11	−0.1911 (4)	0.4196 (2)	−0.1412 (3)	0.0977 (10)
C5′	0.9152 (4)	0.71857 (15)	0.6162 (5)	0.1008 (12)
C10	−0.1889 (4)	0.47476 (19)	−0.0920 (3)	0.0913 (9)
C6′	0.9762 (5)	0.68936 (17)	0.7222 (4)	0.1071 (12)
C7′	0.8736 (4)	0.65473 (17)	0.7664 (3)	0.0969 (10)
H5A	−0.448 (4)	0.5694 (12)	0.403 (3)	0.082 (8)*
H10′	0.394 (3)	0.6541 (11)	0.559 (2)	0.070 (7)*
H6A	−0.540 (4)	0.4903 (11)	0.280 (2)	0.076 (7)*
H5B	−0.448 (3)	0.5927 (11)	0.277 (2)	0.071 (7)*
H6B	−0.355 (3)	0.4734 (12)	0.365 (2)	0.071 (7)*
H8′	0.629 (5)	0.6273 (16)	0.736 (3)	0.125 (12)*
H10	−0.146 (4)	0.5098 (15)	−0.128 (3)	0.112 (11)*
H13	−0.341 (4)	0.3442 (15)	0.041 (3)	0.096 (10)*
H9	−0.246 (4)	0.5203 (15)	0.043 (3)	0.095 (10)*
H1′	0.180 (4)	0.6777 (16)	0.382 (3)	0.107 (11)*
H2	0.134 (4)	0.5959 (12)	0.575 (3)	0.083 (8)*
H4A	−0.132 (5)	0.6636 (18)	0.200 (3)	0.122 (13)*
H3′	0.751 (4)	0.7664 (16)	0.413 (3)	0.113 (10)*
H6′	1.104 (5)	0.6919 (18)	0.771 (3)	0.133 (13)*
H12	−0.249 (5)	0.3291 (18)	−0.124 (3)	0.124 (12)*
H4B	−0.267 (5)	0.6107 (19)	0.157 (4)	0.138 (14)*
H11	−0.150 (4)	0.4097 (16)	−0.213 (3)	0.120 (11)*
H2′	0.458 (4)	0.7552 (16)	0.306 (3)	0.102 (11)*

H4C	−0.304 (6)	0.670 (2)	0.212 (4)	0.148 (15)*
H5′	0.974 (4)	0.7413 (15)	0.573 (3)	0.104 (10)*
H7′	0.937 (6)	0.634 (2)	0.855 (5)	0.170 (18)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0638 (9)	0.0724 (10)	0.0572 (8)	−0.0028 (7)	0.0280 (7)	0.0008 (7)
O2	0.0876 (13)	0.1041 (14)	0.0733 (11)	−0.0111 (10)	0.0431 (10)	0.0035 (9)
N1	0.0562 (9)	0.0573 (10)	0.0581 (10)	0.0053 (8)	0.0221 (8)	0.0002 (8)
O1	0.0934 (13)	0.0978 (14)	0.0590 (10)	0.0078 (10)	0.0177 (9)	0.0115 (9)
O1′	0.0843 (13)	0.0958 (14)	0.0938 (13)	0.0026 (10)	0.0305 (11)	0.0253 (11)
N3	0.0746 (13)	0.0691 (12)	0.0586 (11)	0.0051 (10)	0.0308 (10)	−0.0026 (9)
O4	0.1245 (16)	0.0762 (11)	0.0852 (12)	−0.0154 (10)	0.0589 (11)	−0.0029 (9)
N2	0.0683 (12)	0.0661 (12)	0.0741 (12)	−0.0026 (9)	0.0287 (10)	0.0014 (9)
C1	0.0613 (12)	0.0563 (11)	0.0538 (11)	0.0060 (9)	0.0226 (9)	0.0004 (9)
C3	0.0694 (14)	0.0577 (12)	0.0677 (13)	0.0034 (10)	0.0286 (11)	0.0043 (10)
C8	0.0571 (12)	0.0904 (17)	0.0500 (11)	0.0015 (11)	0.0173 (9)	−0.0006 (10)
C2	0.0649 (14)	0.0645 (13)	0.0660 (14)	0.0048 (11)	0.0219 (11)	−0.0037 (11)
C7	0.0619 (13)	0.0732 (15)	0.0581 (12)	−0.0052 (11)	0.0239 (10)	−0.0017 (10)
C10′	0.0707 (14)	0.0613 (13)	0.0796 (15)	−0.0055 (11)	0.0368 (12)	−0.0040 (11)
C5	0.0541 (12)	0.0740 (15)	0.0679 (14)	0.0079 (11)	0.0230 (11)	0.0019 (11)
C9′	0.0758 (15)	0.0580 (13)	0.0816 (16)	−0.0034 (11)	0.0381 (12)	−0.0181 (11)
C1′	0.0757 (16)	0.0597 (13)	0.0914 (17)	0.0017 (11)	0.0390 (14)	0.0034 (12)
C6	0.0593 (13)	0.0755 (15)	0.0585 (13)	−0.0031 (11)	0.0278 (10)	−0.0014 (11)
C9	0.0732 (15)	0.103 (2)	0.0595 (14)	−0.0112 (14)	0.0272 (12)	−0.0008 (13)
C4′	0.0784 (17)	0.0543 (13)	0.121 (2)	−0.0065 (12)	0.0508 (16)	−0.0169 (14)
C4	0.094 (2)	0.088 (2)	0.0754 (17)	−0.0009 (18)	0.0263 (16)	0.0244 (15)
C13	0.0924 (19)	0.094 (2)	0.0640 (15)	0.0123 (16)	0.0245 (14)	−0.0047 (14)
C8′	0.0856 (18)	0.0873 (19)	0.0835 (18)	−0.0045 (15)	0.0306 (15)	−0.0211 (15)
C2′	0.106 (2)	0.0732 (17)	0.113 (2)	0.0034 (16)	0.057 (2)	0.0197 (17)
C3′	0.096 (2)	0.0680 (17)	0.157 (3)	−0.0086 (15)	0.075 (2)	0.0096 (18)
C12	0.103 (2)	0.123 (3)	0.0663 (16)	0.030 (2)	0.0229 (16)	−0.0136 (17)
C11	0.0785 (18)	0.157 (3)	0.0607 (16)	0.0163 (19)	0.0268 (13)	0.0002 (19)
C5′	0.083 (2)	0.0666 (17)	0.168 (4)	−0.0161 (15)	0.062 (2)	−0.032 (2)
C10	0.0742 (17)	0.140 (3)	0.0655 (16)	−0.0110 (17)	0.0302 (13)	0.0037 (18)
C6′	0.085 (2)	0.088 (2)	0.138 (3)	−0.0008 (18)	0.021 (2)	−0.042 (2)
C7′	0.0807 (19)	0.100 (2)	0.104 (2)	−0.0034 (17)	0.0213 (17)	−0.0365 (19)

Geometric parameters (Å, º)

O3—C7	1.339 (3)	C1′—C2′	1.417 (4)
O3—C6	1.448 (3)	C6—H6A	1.02 (3)
O2—N3	1.221 (3)	C6—H6B	0.96 (3)
N1—C1	1.385 (3)	C9—C10	1.395 (4)
N1—C3	1.352 (3)	C9—H9	0.96 (3)
N1—C5	1.468 (3)	C4′—C3′	1.393 (5)
O1—N3	1.234 (3)	C4′—C5′	1.447 (5)

O1′—C1′	1.356 (3)	C4—H4A	0.88 (4)
O1′—H1′	0.91 (4)	C4—H4B	1.02 (5)
N3—C1	1.416 (3)	C4—H4C	1.00 (5)
O4—C7	1.202 (3)	C13—C12	1.395 (4)
N2—C3	1.332 (3)	C13—H13	0.98 (3)
N2—C2	1.351 (3)	C8′—C7′	1.364 (4)
C1—C2	1.352 (3)	C8′—H8′	1.02 (4)
C3—C4	1.484 (4)	C2′—C3′	1.348 (5)
C8—C7	1.488 (3)	C2′—H2′	0.87 (3)
C8—C9	1.371 (4)	C3′—H3′	0.95 (4)
C8—C13	1.386 (4)	C12—C11	1.372 (5)
C2—H2	0.93 (3)	C12—H12	1.00 (4)
C10′—C9′	1.419 (4)	C11—C10	1.362 (5)
C10′—C1′	1.361 (4)	C11—H11	1.04 (4)
C10′—H10′	0.95 (3)	C5′—C6′	1.356 (6)
C5—C6	1.492 (3)	C5′—H5′	0.96 (3)
C5—H5A	0.95 (3)	C10—H10	1.01 (4)
C5—H5B	0.99 (3)	C6′—C7′	1.388 (6)
C9′—C4′	1.406 (4)	C6′—H6′	1.05 (4)
C9′—C8′	1.418 (4)	C7′—H7′	1.11 (5)

C7—O3—C6	114.89 (17)	H6A—C6—H6B	109 (2)
C1—N1—C5	128.84 (19)	C8—C9—C10	120.4 (3)
C3—N1—C1	105.12 (18)	C8—C9—H9	117.6 (19)
C3—N1—C5	126.04 (19)	C10—C9—H9	122 (2)
C1′—O1′—H1′	112 (2)	C9′—C4′—C5′	117.7 (3)
O2—N3—O1	123.6 (2)	C3′—C4′—C9′	118.7 (3)
O2—N3—C1	119.8 (2)	C3′—C4′—C5′	123.5 (3)
O1—N3—C1	116.5 (2)	C3—C4—H4A	109 (3)
C3—N2—C2	105.8 (2)	C3—C4—H4B	111 (2)
N1—C1—N3	125.74 (19)	C3—C4—H4C	112 (3)
C2—C1—N1	107.28 (19)	H4A—C4—H4B	116 (3)
C2—C1—N3	127.0 (2)	H4A—C4—H4C	107 (4)
N1—C3—C4	124.1 (2)	H4B—C4—H4C	101 (4)
N2—C3—N1	111.9 (2)	C8—C13—C12	119.5 (3)
N2—C3—C4	124.0 (2)	C8—C13—H13	117.7 (19)
C9—C8—C7	122.8 (2)	C12—C13—H13	122.7 (19)
C9—C8—C13	119.7 (2)	C9′—C8′—H8′	116 (2)
C13—C8—C7	117.5 (2)	C7′—C8′—C9′	121.7 (3)
N2—C2—C1	109.9 (2)	C7′—C8′—H8′	122 (2)
N2—C2—H2	121.8 (18)	C1′—C2′—H2′	113 (2)
C1—C2—H2	128.3 (18)	C3′—C2′—C1′	120.5 (3)
O3—C7—C8	113.3 (2)	C3′—C2′—H2′	126 (2)
O4—C7—O3	122.5 (2)	C4′—C3′—H3′	113 (2)
O4—C7—C8	124.2 (2)	C2′—C3′—C4′	121.7 (3)
C9′—C10′—H10′	119.9 (15)	C2′—C3′—H3′	125 (2)
C1′—C10′—C9′	120.9 (2)	C13—C12—H12	115 (2)
C1′—C10′—H10′	119.1 (15)	C11—C12—C13	120.0 (3)

N1—C5—C6	113.15 (19)	C11—C12—H12	125 (2)
N1—C5—H5A	107.8 (17)	C12—C11—H11	114 (2)
N1—C5—H5B	106.3 (14)	C10—C11—C12	120.6 (3)
C6—C5—H5A	108.5 (17)	C10—C11—H11	125 (2)
C6—C5—H5B	113.1 (14)	C4′—C5′—H5′	110 (2)
H5A—C5—H5B	108 (2)	C6′—C5′—C4′	121.0 (3)
C4′—C9′—C10′	119.0 (3)	C6′—C5′—H5′	129 (2)
C4′—C9′—C8′	118.8 (3)	C9—C10—H10	121 (2)
C8′—C9′—C10′	122.2 (2)	C11—C10—C9	119.8 (3)
O1′—C1′—C10′	124.8 (2)	C11—C10—H10	119 (2)
O1′—C1′—C2′	116.1 (3)	C5′—C6′—C7′	120.9 (4)
C10′—C1′—C2′	119.1 (3)	C5′—C6′—H6′	120 (2)
O3—C6—C5	108.53 (19)	C7′—C6′—H6′	119 (2)
O3—C6—H6A	110.0 (15)	C8′—C7′—C6′	119.9 (4)
O3—C6—H6B	109.4 (15)	C8′—C7′—H7′	126 (3)
C5—C6—H6A	107.5 (14)	C6′—C7′—H7′	114 (3)
C5—C6—H6B	112.5 (15)		

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–4-methoxybenzoic acid (1/1) (bzmdmac)

Crystal data

$C_{13}H_{13}N_3O_4{\cdot}C_8H_8O_3$
$M_r = 427.41$
Triclinic, $P\overline{1}$
$a = 9.1309$ (4) Å
$b = 11.1274$ (4) Å
$c = 11.8538$ (5) Å
$\alpha = 107.365$ (1)°
$\beta = 103.270$ (1)°
$\gamma = 110.091$ (1)°
$V = 1002.73$ (7) Å^3
$Z = 2$
$F(000) = 448$
$D_x = 1.416$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9919 reflections
$\theta = 2.5$–27.5°
$\mu = 0.11$ mm^{-1}
$T = 300$ K
Plate, clear light colourless
0.73 × 0.49 × 0.21 mm

Data collection

Bruker APEX3 microsource diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.587$, $T_{max} = 0.746$
32021 measured reflections
4583 independent reflections
3795 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.6°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.165$
$S = 1.05$
4583 reflections
364 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0785P)^2 + 0.4129P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.25372 (18)	0.92488 (15)	0.54618 (12)	0.0501 (3)
O1′	0.8663 (2)	0.60162 (19)	0.82192 (14)	0.0593 (4)
O3′	1.3864 (2)	0.35358 (17)	0.84208 (14)	0.0603 (4)
O2′	0.8625 (2)	0.56494 (18)	0.62520 (14)	0.0617 (4)
O4	0.3621 (2)	0.82888 (18)	0.41261 (14)	0.0592 (4)
O2	0.2647 (2)	0.86239 (18)	0.88018 (15)	0.0624 (4)
O1	0.4097 (2)	0.84360 (19)	1.03975 (14)	0.0675 (5)
N1	0.43006 (18)	0.75915 (15)	0.73271 (14)	0.0395 (3)
N3	0.3715 (2)	0.83160 (16)	0.92979 (14)	0.0442 (4)
N2	0.63325 (19)	0.70185 (17)	0.79998 (15)	0.0463 (4)
C2′	1.0933 (2)	0.44853 (18)	0.66222 (16)	0.0404 (4)
C1′	1.0392 (2)	0.50531 (17)	0.75630 (15)	0.0372 (4)
C8	0.1692 (2)	0.91266 (18)	0.33808 (16)	0.0395 (4)
C5	0.3002 (2)	0.76950 (19)	0.64032 (17)	0.0423 (4)
C3′	1.2086 (2)	0.39608 (19)	0.68643 (17)	0.0420 (4)
C3	0.4572 (2)	0.77942 (18)	0.85787 (16)	0.0391 (4)
C4′	1.2720 (2)	0.40079 (19)	0.80701 (17)	0.0418 (4)
C7	0.2705 (2)	0.88207 (19)	0.43220 (17)	0.0420 (4)
C1	0.5419 (2)	0.71451 (18)	0.70306 (17)	0.0403 (4)
C7′	0.9147 (2)	0.55954 (19)	0.72677 (17)	0.0422 (4)
C6′	1.1052 (2)	0.5099 (2)	0.87698 (17)	0.0434 (4)
C2	0.5799 (2)	0.7421 (2)	0.89668 (18)	0.0460 (4)
C6	0.3670 (3)	0.9180 (2)	0.64893 (18)	0.0482 (4)
C4	0.5590 (3)	0.6836 (3)	0.5775 (2)	0.0540 (5)
C5′	1.2197 (3)	0.4587 (2)	0.90209 (18)	0.0474 (4)
C9	0.1616 (3)	0.8622 (2)	0.21389 (18)	0.0508 (5)
C8′	1.4517 (4)	0.2998 (3)	0.7517 (3)	0.0650 (6)
C13	0.0911 (3)	0.9973 (3)	0.3722 (2)	0.0545 (5)
C11	−0.0037 (3)	0.9767 (3)	0.1587 (2)	0.0651 (6)
C10	0.0749 (3)	0.8943 (3)	0.1246 (2)	0.0639 (6)
C12	0.0049 (3)	1.0293 (3)	0.2823 (3)	0.0670 (6)
H5A	0.269 (3)	0.702 (2)	0.552 (2)	0.046 (5)*

H5B	0.194 (3)	0.744 (2)	0.6573 (19)	0.041 (5)*
H6A	0.480 (3)	0.942 (2)	0.640 (2)	0.055 (6)*
H6B	0.373 (3)	0.985 (2)	0.734 (2)	0.054 (6)*
H6′	1.069 (3)	0.549 (2)	0.941 (2)	0.062 (6)*
H2′	1.055 (3)	0.446 (2)	0.578 (2)	0.051 (6)*
H4A	0.645 (3)	0.659 (2)	0.577 (2)	0.056 (6)*
H2	0.624 (3)	0.739 (3)	0.977 (3)	0.070 (7)*
H3′	1.243 (3)	0.357 (2)	0.620 (2)	0.062 (7)*
H5′	1.261 (3)	0.460 (3)	0.983 (3)	0.071 (7)*
H8′A	1.509 (4)	0.375 (3)	0.726 (3)	0.081 (8)*
H9	0.219 (3)	0.804 (3)	0.190 (2)	0.069 (7)*
H13	0.095 (3)	1.031 (3)	0.451 (3)	0.066 (7)*
H4B	0.458 (4)	0.606 (3)	0.509 (3)	0.090 (9)*
H1′	0.798 (4)	0.636 (3)	0.811 (3)	0.086 (9)*
H4C	0.579 (4)	0.759 (3)	0.556 (3)	0.084 (9)*
H8′B	1.362 (4)	0.219 (3)	0.681 (3)	0.088 (9)*
H8′C	1.527 (4)	0.271 (3)	0.796 (3)	0.079 (8)*
H10	0.069 (4)	0.855 (3)	0.037 (3)	0.096 (9)*
H12	−0.045 (4)	1.088 (3)	0.313 (3)	0.095 (10)*
H11	−0.073 (4)	0.990 (3)	0.088 (3)	0.082 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0631 (8)	0.0679 (8)	0.0405 (7)	0.0422 (7)	0.0235 (6)	0.0306 (6)
O1′	0.0634 (9)	0.0923 (11)	0.0499 (8)	0.0555 (9)	0.0293 (7)	0.0337 (8)
O3′	0.0698 (9)	0.0814 (10)	0.0511 (8)	0.0548 (8)	0.0214 (7)	0.0307 (7)
O2′	0.0699 (9)	0.0916 (11)	0.0458 (8)	0.0558 (9)	0.0213 (7)	0.0333 (8)
O4	0.0709 (9)	0.0877 (10)	0.0554 (8)	0.0566 (9)	0.0350 (7)	0.0419 (8)
O2	0.0763 (10)	0.0866 (11)	0.0602 (9)	0.0601 (9)	0.0375 (8)	0.0386 (8)
O1	0.0819 (11)	0.0950 (12)	0.0368 (7)	0.0490 (10)	0.0272 (7)	0.0260 (8)
N1	0.0455 (7)	0.0473 (8)	0.0370 (7)	0.0274 (6)	0.0182 (6)	0.0213 (6)
N3	0.0501 (8)	0.0473 (8)	0.0407 (8)	0.0245 (7)	0.0208 (7)	0.0187 (6)
N2	0.0451 (8)	0.0586 (9)	0.0472 (8)	0.0310 (7)	0.0185 (7)	0.0265 (7)
C2′	0.0439 (9)	0.0471 (9)	0.0325 (8)	0.0221 (7)	0.0136 (7)	0.0177 (7)
C1′	0.0361 (8)	0.0417 (8)	0.0364 (8)	0.0177 (6)	0.0144 (6)	0.0178 (7)
C8	0.0384 (8)	0.0490 (9)	0.0381 (8)	0.0209 (7)	0.0165 (7)	0.0235 (7)
C5	0.0425 (9)	0.0461 (9)	0.0400 (9)	0.0214 (7)	0.0145 (7)	0.0187 (7)
C3′	0.0480 (9)	0.0476 (9)	0.0355 (8)	0.0257 (8)	0.0183 (7)	0.0162 (7)
C3	0.0433 (8)	0.0438 (8)	0.0353 (8)	0.0216 (7)	0.0163 (7)	0.0186 (7)
C4′	0.0427 (9)	0.0462 (9)	0.0405 (9)	0.0240 (7)	0.0133 (7)	0.0194 (7)
C7	0.0463 (9)	0.0523 (9)	0.0405 (9)	0.0277 (8)	0.0205 (7)	0.0256 (8)
C1	0.0431 (9)	0.0440 (9)	0.0417 (9)	0.0237 (7)	0.0192 (7)	0.0201 (7)
C7′	0.0397 (8)	0.0483 (9)	0.0399 (9)	0.0215 (7)	0.0150 (7)	0.0174 (7)
C6′	0.0461 (9)	0.0562 (10)	0.0371 (9)	0.0265 (8)	0.0211 (7)	0.0226 (8)
C2	0.0468 (9)	0.0588 (11)	0.0402 (9)	0.0285 (8)	0.0152 (7)	0.0249 (8)
C6	0.0546 (11)	0.0501 (10)	0.0388 (9)	0.0232 (8)	0.0120 (8)	0.0209 (8)
C4	0.0650 (13)	0.0688 (13)	0.0497 (11)	0.0431 (11)	0.0311 (10)	0.0287 (10)

C5′	0.0550 (10)	0.0630 (11)	0.0346 (9)	0.0320 (9)	0.0178 (8)	0.0254 (8)
C9	0.0606 (11)	0.0591 (11)	0.0383 (9)	0.0316 (10)	0.0186 (8)	0.0209 (8)
C8′	0.0742 (15)	0.0746 (15)	0.0626 (14)	0.0540 (14)	0.0248 (12)	0.0250 (12)
C13	0.0622 (12)	0.0804 (14)	0.0480 (11)	0.0464 (11)	0.0302 (9)	0.0363 (10)
C11	0.0629 (13)	0.0952 (17)	0.0603 (13)	0.0452 (13)	0.0218 (11)	0.0504 (13)
C10	0.0773 (15)	0.0840 (15)	0.0384 (10)	0.0415 (13)	0.0187 (10)	0.0308 (10)
C12	0.0744 (15)	0.0998 (18)	0.0706 (15)	0.0638 (14)	0.0384 (12)	0.0524 (14)

Geometric parameters (Å, º)

O3—C7	1.355 (2)	C3′—C4′	1.391 (2)
O3—C6	1.446 (2)	C3′—H3′	0.96 (3)
O1′—C7′	1.320 (2)	C3—C2	1.355 (2)
O1′—H1′	0.84 (3)	C4′—C5′	1.392 (3)
O3′—C4′	1.359 (2)	C1—C4	1.482 (3)
O3′—C8′	1.421 (3)	C6′—C5′	1.369 (3)
O2′—C7′	1.217 (2)	C6′—H6′	0.94 (3)
O4—C7	1.204 (2)	C2—H2	0.97 (3)
O2—N3	1.225 (2)	C6—H6A	1.01 (2)
O1—N3	1.222 (2)	C6—H6B	1.04 (2)
N1—C5	1.480 (2)	C4—H4A	0.92 (3)
N1—C3	1.381 (2)	C4—H4B	0.97 (3)
N1—C1	1.350 (2)	C4—H4C	0.92 (3)
N3—C3	1.414 (2)	C5′—H5′	0.94 (3)
N2—C1	1.331 (2)	C9—C10	1.382 (3)
N2—C2	1.361 (2)	C9—H9	0.98 (3)
C2′—C1′	1.391 (2)	C8′—H8′A	1.00 (3)
C2′—C3′	1.384 (2)	C8′—H8′B	0.95 (3)
C2′—H2′	0.97 (2)	C8′—H8′C	0.98 (3)
C1′—C7′	1.481 (2)	C13—C12	1.384 (3)
C1′—C6′	1.397 (2)	C13—H13	0.88 (3)
C8—C7	1.478 (2)	C11—C10	1.372 (4)
C8—C9	1.386 (3)	C11—C12	1.379 (4)
C8—C13	1.388 (3)	C11—H11	1.01 (3)
C5—C6	1.513 (3)	C10—H10	0.98 (3)
C5—H5A	1.00 (2)	C12—H12	0.95 (3)
C5—H5B	1.00 (2)		

C7—O3—C6	115.93 (14)	C1′—C6′—H6′	118.4 (15)
C7′—O1′—H1′	117 (2)	C5′—C6′—C1′	120.87 (17)
C4′—O3′—C8′	118.47 (17)	C5′—C6′—H6′	120.7 (15)
C3—N1—C5	130.29 (14)	N2—C2—H2	122.3 (16)
C1—N1—C5	123.92 (15)	C3—C2—N2	109.30 (16)
C1—N1—C3	105.61 (14)	C3—C2—H2	128.3 (16)
O2—N3—C3	119.27 (15)	O3—C6—C5	109.66 (15)
O1—N3—O2	123.58 (16)	O3—C6—H6A	109.6 (13)
O1—N3—C3	117.15 (16)	O3—C6—H6B	107.7 (12)
C1—N2—C2	106.00 (15)	C5—C6—H6A	107.2 (12)

C1′—C2′—H2′	121.8 (13)	C5—C6—H6B	109.6 (12)
C3′—C2′—C1′	121.08 (16)	H6A—C6—H6B	113.0 (18)
C3′—C2′—H2′	117.1 (13)	C1—C4—H4A	110.3 (15)
C2′—C1′—C7′	119.62 (15)	C1—C4—H4B	112.5 (18)
C2′—C1′—C6′	118.55 (16)	C1—C4—H4C	111.9 (19)
C6′—C1′—C7′	121.83 (16)	H4A—C4—H4B	107 (2)
C9—C8—C7	118.52 (16)	H4A—C4—H4C	109 (2)
C9—C8—C13	119.36 (17)	H4B—C4—H4C	106 (3)
C13—C8—C7	121.99 (16)	C4′—C5′—H5′	119.7 (16)
N1—C5—C6	108.80 (15)	C6′—C5′—C4′	120.21 (17)
N1—C5—H5A	111.9 (12)	C6′—C5′—H5′	120.1 (16)
N1—C5—H5B	111.0 (11)	C8—C9—H9	119.7 (15)
C6—C5—H5A	109.4 (12)	C10—C9—C8	120.3 (2)
C6—C5—H5B	110.5 (11)	C10—C9—H9	120.1 (15)
H5A—C5—H5B	105.3 (16)	O3′—C8′—H8′A	108.8 (17)
C2′—C3′—C4′	119.46 (16)	O3′—C8′—H8′B	108.8 (19)
C2′—C3′—H3′	119.6 (15)	O3′—C8′—H8′C	104.0 (17)
C4′—C3′—H3′	120.9 (15)	H8′A—C8′—H8′B	111 (3)
N1—C3—N3	124.90 (15)	H8′A—C8′—H8′C	114 (2)
C2—C3—N1	107.41 (15)	H8′B—C8′—H8′C	109 (2)
C2—C3—N3	127.68 (16)	C8—C13—H13	120.7 (17)
O3′—C4′—C3′	124.69 (17)	C12—C13—C8	120.1 (2)
O3′—C4′—C5′	115.47 (16)	C12—C13—H13	119.3 (17)
C3′—C4′—C5′	119.83 (16)	C10—C11—C12	120.4 (2)
O3—C7—C8	112.45 (14)	C10—C11—H11	116.3 (16)
O4—C7—O3	122.94 (16)	C12—C11—H11	123.2 (17)
O4—C7—C8	124.57 (16)	C9—C10—H10	118.5 (19)
N1—C1—C4	123.52 (16)	C11—C10—C9	120.0 (2)
N2—C1—N1	111.65 (15)	C11—C10—H10	121.4 (19)
N2—C1—C4	124.83 (16)	C13—C12—H12	115 (2)
O1′—C7′—C1′	113.17 (15)	C11—C12—C13	119.9 (2)
O2′—C7′—O1′	123.39 (17)	C11—C12—H12	125 (2)
O2′—C7′—C1′	123.44 (16)		

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–3,5-dinitrobenzoic acid (1/1) (bzmd35dnz)

Crystal data

$C_{13}H_{13}N_3O_4·C_7H_4N_2O_6$	$F(000) = 1008$
$M_r = 487.39$	$D_x = 1.533$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 21.0988$ (13) Å	Cell parameters from 9941 reflections
$b = 8.4322$ (5) Å	$\theta = 2.6$–$27.3°$
$c = 12.0341$ (8) Å	$\mu = 0.13$ mm^{-1}
$\beta = 99.505$ (2)°	$T = 300$ K
$V = 2111.6$ (2) Å^3	Plate, clear light colourless
$Z = 4$	0.46 × 0.40 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.587, T_{max} = 0.746
71598 measured reflections
4820 independent reflections
3321 reflections with $I > 2\sigma(I)$
R_{int} = 0.108
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −27→27
k = −10→10
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.213
S = 1.14
4820 reflections
385 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0808P)^2 + 2.0317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.026 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.88887 (9)	0.4296 (3)	0.67819 (18)	0.0501 (5)
O1′	0.62334 (9)	0.4206 (3)	0.8640 (2)	0.0519 (6)
O6′	0.41665 (11)	0.3221 (3)	0.9795 (2)	0.0617 (7)
O2′	0.62851 (10)	0.6000 (3)	0.7300 (2)	0.0691 (8)
N1	0.84690 (10)	0.3243 (3)	0.8853 (2)	0.0403 (5)
O3′	0.42660 (12)	0.6852 (3)	0.4624 (2)	0.0659 (7)
O5′	0.32969 (10)	0.4181 (4)	0.8826 (2)	0.0672 (7)
O4′	0.33601 (11)	0.6115 (4)	0.5067 (2)	0.0731 (8)
N2	0.74971 (11)	0.4037 (3)	0.9065 (2)	0.0485 (6)
N1′	0.38764 (11)	0.3936 (3)	0.8979 (2)	0.0500 (6)
O2	0.95921 (11)	0.3723 (4)	1.0441 (2)	0.0787 (9)
O4	0.97119 (11)	0.5544 (4)	0.6211 (3)	0.0766 (8)
N3	0.90992 (12)	0.4399 (4)	1.0593 (2)	0.0521 (7)
O1	0.90695 (14)	0.5286 (4)	1.1385 (2)	0.0810 (9)

N2′	0.39462 (13)	0.6237 (3)	0.5270 (2)	0.0533 (7)
C5′	0.52600 (12)	0.5108 (3)	0.7595 (3)	0.0419 (6)
C1′	0.42448 (12)	0.4538 (3)	0.8136 (3)	0.0419 (6)
C4′	0.49473 (13)	0.5679 (3)	0.6577 (3)	0.0437 (7)
C6′	0.49130 (13)	0.4515 (4)	0.8391 (3)	0.0427 (7)
C1	0.78368 (13)	0.3235 (4)	0.8418 (3)	0.0434 (7)
C3′	0.42799 (13)	0.5640 (3)	0.6359 (3)	0.0436 (7)
C3	0.85199 (13)	0.4118 (4)	0.9835 (2)	0.0424 (6)
C7′	0.59800 (13)	0.5155 (4)	0.7827 (3)	0.0461 (7)
C2′	0.39175 (13)	0.5094 (4)	0.7128 (3)	0.0454 (7)
C7	0.91451 (14)	0.5258 (4)	0.6079 (3)	0.0493 (7)
C8	0.86719 (15)	0.5910 (4)	0.5147 (3)	0.0482 (7)
C5	0.89796 (15)	0.2510 (4)	0.8332 (3)	0.0493 (7)
C6	0.93347 (15)	0.3681 (5)	0.7725 (3)	0.0523 (8)
C2	0.79212 (14)	0.4589 (4)	0.9961 (3)	0.0480 (7)
C11	0.7809 (2)	0.7221 (5)	0.3390 (4)	0.0706 (11)
C4	0.75565 (19)	0.2433 (6)	0.7357 (4)	0.0639 (10)
C10	0.75929 (19)	0.6644 (5)	0.4327 (4)	0.0685 (10)
C9	0.80146 (16)	0.5962 (4)	0.5207 (3)	0.0569 (8)
C13	0.8889 (2)	0.6517 (4)	0.4218 (3)	0.0613 (9)
C12	0.8460 (2)	0.7149 (5)	0.3335 (3)	0.0718 (11)
H4′	0.5171 (15)	0.612 (4)	0.593 (3)	0.046 (8)*
H2′	0.3449 (16)	0.512 (4)	0.695 (3)	0.041 (8)*
H5A	0.8774 (17)	0.173 (4)	0.780 (3)	0.057 (10)*
H6′	0.5098 (15)	0.409 (4)	0.912 (3)	0.044 (8)*
H5B	0.9296 (17)	0.201 (4)	0.897 (3)	0.059 (10)*
H2	0.7782 (19)	0.516 (5)	1.051 (3)	0.066 (11)*
H6A	0.9522 (16)	0.454 (4)	0.825 (3)	0.049 (9)*
H9	0.7866 (16)	0.548 (4)	0.590 (3)	0.047 (9)*
H1′	0.671 (2)	0.429 (5)	0.882 (3)	0.073 (12)*
H6B	0.9718 (18)	0.319 (4)	0.747 (3)	0.060 (10)*
H13	0.935 (2)	0.639 (6)	0.419 (4)	0.089 (14)*
H10	0.714 (2)	0.669 (5)	0.439 (4)	0.084 (13)*
H12	0.866 (2)	0.751 (6)	0.265 (5)	0.110 (17)*
H11	0.7488 (19)	0.769 (5)	0.276 (3)	0.067 (11)*
H4A	0.759 (2)	0.131 (7)	0.751 (4)	0.104 (17)*
H4B	0.773 (2)	0.282 (5)	0.668 (4)	0.072 (12)*
H4C	0.711 (3)	0.267 (6)	0.716 (4)	0.099 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0329 (10)	0.0680 (14)	0.0492 (12)	−0.0043 (9)	0.0063 (8)	0.0048 (10)
O1′	0.0273 (9)	0.0594 (13)	0.0677 (14)	0.0030 (9)	0.0035 (9)	0.0137 (11)
O6′	0.0479 (12)	0.0870 (18)	0.0510 (13)	0.0040 (12)	0.0107 (10)	−0.0001 (12)
O2′	0.0353 (11)	0.0812 (17)	0.0884 (19)	−0.0069 (11)	0.0032 (11)	0.0323 (15)
N1	0.0306 (11)	0.0462 (13)	0.0442 (13)	0.0038 (9)	0.0064 (9)	0.0033 (10)
O3′	0.0580 (14)	0.0854 (18)	0.0528 (14)	0.0023 (13)	0.0047 (11)	0.0062 (13)

O5′	0.0304 (11)	0.099 (2)	0.0742 (17)	0.0064 (11)	0.0144 (10)	−0.0028 (14)
O4′	0.0410 (12)	0.095 (2)	0.0752 (18)	−0.0037 (12)	−0.0136 (12)	0.0065 (15)
N2	0.0296 (11)	0.0577 (15)	0.0581 (16)	0.0034 (10)	0.0075 (11)	0.0069 (12)
N1′	0.0341 (12)	0.0632 (16)	0.0539 (16)	0.0018 (11)	0.0107 (11)	−0.0132 (13)
O2	0.0378 (12)	0.124 (2)	0.0699 (17)	0.0138 (14)	−0.0042 (11)	−0.0054 (16)
O4	0.0367 (12)	0.104 (2)	0.089 (2)	−0.0152 (13)	0.0115 (12)	0.0193 (16)
N3	0.0404 (13)	0.0696 (18)	0.0443 (15)	−0.0002 (12)	0.0013 (11)	0.0053 (13)
O1	0.0725 (18)	0.109 (2)	0.0557 (16)	0.0028 (16)	−0.0065 (13)	−0.0216 (16)
N2′	0.0437 (14)	0.0577 (16)	0.0536 (16)	0.0041 (12)	−0.0061 (12)	−0.0073 (13)
C5′	0.0296 (12)	0.0395 (14)	0.0551 (17)	0.0026 (10)	0.0029 (11)	−0.0038 (13)
C1′	0.0292 (12)	0.0481 (15)	0.0481 (16)	0.0014 (11)	0.0054 (11)	−0.0098 (12)
C4′	0.0327 (13)	0.0443 (15)	0.0529 (17)	0.0021 (11)	0.0033 (12)	−0.0045 (13)
C6′	0.0321 (13)	0.0448 (15)	0.0498 (17)	0.0014 (11)	0.0024 (12)	−0.0065 (13)
C1	0.0313 (13)	0.0468 (15)	0.0514 (16)	−0.0034 (11)	0.0048 (11)	0.0044 (13)
C3′	0.0355 (14)	0.0448 (15)	0.0480 (16)	0.0046 (11)	0.0001 (12)	−0.0053 (12)
C3	0.0347 (13)	0.0499 (16)	0.0420 (15)	0.0029 (11)	0.0042 (11)	0.0082 (12)
C7′	0.0333 (13)	0.0466 (16)	0.0569 (18)	−0.0009 (12)	0.0029 (12)	0.0028 (14)
C2′	0.0305 (13)	0.0500 (16)	0.0542 (17)	0.0036 (11)	0.0027 (12)	−0.0101 (14)
C7	0.0379 (14)	0.0588 (18)	0.0526 (18)	−0.0064 (13)	0.0118 (13)	−0.0055 (14)
C8	0.0451 (15)	0.0503 (17)	0.0493 (17)	−0.0048 (13)	0.0079 (13)	−0.0066 (13)
C5	0.0384 (15)	0.0557 (18)	0.0552 (18)	0.0062 (13)	0.0119 (13)	0.0000 (15)
C6	0.0348 (14)	0.072 (2)	0.0505 (18)	0.0036 (14)	0.0081 (13)	0.0011 (16)
C2	0.0408 (15)	0.0587 (18)	0.0456 (17)	0.0085 (13)	0.0100 (13)	0.0043 (14)
C11	0.081 (3)	0.055 (2)	0.067 (2)	0.0016 (19)	−0.013 (2)	−0.0025 (18)
C4	0.050 (2)	0.077 (3)	0.061 (2)	−0.0153 (18)	0.0006 (16)	−0.0085 (19)
C10	0.052 (2)	0.063 (2)	0.085 (3)	−0.0061 (17)	−0.0068 (19)	−0.006 (2)
C9	0.0441 (17)	0.0586 (19)	0.066 (2)	−0.0098 (14)	0.0048 (15)	−0.0023 (17)
C13	0.065 (2)	0.059 (2)	0.063 (2)	0.0035 (17)	0.0208 (18)	0.0003 (17)
C12	0.103 (3)	0.058 (2)	0.055 (2)	0.007 (2)	0.016 (2)	0.0025 (17)

Geometric parameters (Å, º)

O3—C7	1.347 (4)	C6′—H6′	0.97 (3)
O3—C6	1.446 (4)	C1—C4	1.478 (5)
O1′—C7′	1.308 (4)	C3′—C2′	1.374 (4)
O1′—H1′	0.99 (4)	C3—C2	1.356 (4)
O6′—N1′	1.227 (4)	C2′—H2′	0.98 (3)
O2′—C7′	1.208 (4)	C7—C8	1.479 (5)
N1—C1	1.350 (3)	C8—C9	1.401 (4)
N1—C3	1.382 (4)	C8—C13	1.375 (5)
N1—C5	1.469 (4)	C5—C6	1.501 (5)
O3′—N2′	1.225 (4)	C5—H5A	0.97 (4)
O5′—N1′	1.223 (3)	C5—H5B	1.02 (4)
O4′—N2′	1.225 (3)	C6—H6A	1.00 (4)
N2—C1	1.328 (4)	C6—H6B	1.00 (4)
N2—C2	1.364 (4)	C2—H2	0.91 (4)
N1′—C1′	1.467 (4)	C11—C10	1.373 (6)
O2—N3	1.226 (4)	C11—C12	1.387 (6)

O4—C7	1.204 (4)	C11—H11	1.01 (4)
N3—O1	1.221 (4)	C4—H4A	0.97 (6)
N3—C3	1.419 (4)	C4—H4B	1.01 (4)
N2′—C3′	1.469 (4)	C4—H4C	0.95 (5)
C5′—C4′	1.379 (4)	C10—C9	1.390 (5)
C5′—C6′	1.391 (4)	C10—H10	0.97 (5)
C5′—C7′	1.499 (4)	C9—H9	1.02 (3)
C1′—C6′	1.393 (4)	C13—C12	1.384 (6)
C1′—C2′	1.375 (4)	C13—H13	0.98 (4)
C4′—C3′	1.390 (4)	C12—H12	1.04 (5)
C4′—H4′	1.05 (3)		

C7—O3—C6	115.6 (2)	O3—C7—C8	114.1 (2)
C7′—O1′—H1′	113 (2)	O4—C7—O3	122.1 (3)
C1—N1—C3	105.5 (2)	O4—C7—C8	123.8 (3)
C1—N1—C5	125.4 (3)	C9—C8—C7	121.5 (3)
C3—N1—C5	129.1 (2)	C13—C8—C7	118.8 (3)
C1—N2—C2	106.9 (2)	C13—C8—C9	119.7 (3)
O6′—N1′—C1′	118.2 (2)	N1—C5—C6	113.0 (3)
O5′—N1′—O6′	123.9 (3)	N1—C5—H5A	107 (2)
O5′—N1′—C1′	117.9 (3)	N1—C5—H5B	107 (2)
O2—N3—C3	119.2 (3)	C6—C5—H5A	109 (2)
O1—N3—O2	123.7 (3)	C6—C5—H5B	108 (2)
O1—N3—C3	117.0 (3)	H5A—C5—H5B	113 (3)
O3′—N2′—C3′	118.5 (3)	O3—C6—C5	107.8 (3)
O4′—N2′—O3′	123.6 (3)	O3—C6—H6A	112.3 (19)
O4′—N2′—C3′	117.9 (3)	O3—C6—H6B	111 (2)
C4′—C5′—C6′	120.5 (3)	C5—C6—H6A	110.1 (19)
C4′—C5′—C7′	118.5 (3)	C5—C6—H6B	112 (2)
C6′—C5′—C7′	120.9 (3)	H6A—C6—H6B	104 (3)
C6′—C1′—N1′	118.4 (3)	N2—C2—H2	121 (2)
C2′—C1′—N1′	118.8 (2)	C3—C2—N2	108.2 (3)
C2′—C1′—C6′	122.8 (3)	C3—C2—H2	131 (3)
C5′—C4′—C3′	118.8 (3)	C10—C11—C12	119.3 (4)
C5′—C4′—H4′	125.4 (18)	C10—C11—H11	119 (2)
C3′—C4′—H4′	115.8 (18)	C12—C11—H11	122 (2)
C5′—C6′—C1′	118.2 (3)	C1—C4—H4A	106 (3)
C5′—C6′—H6′	125.2 (18)	C1—C4—H4B	114 (2)
C1′—C6′—H6′	116.6 (19)	C1—C4—H4C	111 (3)
N1—C1—C4	124.5 (3)	H4A—C4—H4B	116 (4)
N2—C1—N1	111.3 (3)	H4A—C4—H4C	107 (4)
N2—C1—C4	124.2 (3)	H4B—C4—H4C	102 (4)
C4′—C3′—N2′	118.8 (3)	C11—C10—C9	121.0 (4)
C2′—C3′—N2′	118.5 (3)	C11—C10—H10	121 (3)
C2′—C3′—C4′	122.7 (3)	C9—C10—H10	118 (3)
N1—C3—N3	125.1 (3)	C8—C9—H9	117.9 (19)
C2—C3—N1	108.0 (3)	C10—C9—C8	119.2 (4)
C2—C3—N3	126.7 (3)	C10—C9—H9	122.9 (19)

O1′—C7′—C5′	113.6 (3)	C8—C13—C12	120.3 (4)
O2′—C7′—O1′	124.5 (3)	C8—C13—H13	117 (3)
O2′—C7′—C5′	122.0 (3)	C12—C13—H13	123 (3)
C1′—C2′—H2′	122.6 (18)	C11—C12—H12	124 (3)
C3′—C2′—C1′	117.0 (3)	C13—C12—C11	120.5 (4)
C3′—C2′—H2′	120.4 (18)	C13—C12—H12	115 (3)

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–3-aminobenzoic acid (1/1) (bzmdabn)

Crystal data

$C_{13}H_{13}N_3O_4{\cdot}C_7H_7NO_2$
M_r = 412.40
Triclinic, $P\overline{1}$
a = 7.9316 (7) Å
b = 11.9585 (12) Å
c = 12.1978 (12) Å
α = 76.362 (3)°
β = 78.927 (3)°
γ = 79.583 (3)°
V = 1092.21 (18) Å^3
Z = 2
$F(000)$ = 432
D_x = 1.254 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6174 reflections
θ = 2.7–29.7°
μ = 0.09 mm^{-1}
T = 300 K
Plate, clear light colourless
0.91 × 0.09 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.587, T_{max} = 0.746
38219 measured reflections
5008 independent reflections
2711 reflections with $I > 2\sigma(I)$
R_{int} = 0.090
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −10→10
k = −15→15
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.168
S = 1.00
5008 reflections
340 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0722P)^2 + 0.2049P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4965 (2)	−0.14226 (17)	0.07569 (17)	0.0875 (6)
O2	0.2393 (2)	−0.07338 (15)	0.03516 (16)	0.0810 (5)
O3	0.13769 (18)	0.29191 (12)	0.00673 (13)	0.0578 (4)
O4	0.1642 (3)	0.33490 (16)	−0.18307 (15)	0.0845 (6)
N1	0.2025 (2)	0.08578 (15)	0.17918 (14)	0.0541 (4)
N2	0.3948 (3)	0.0924 (2)	0.28556 (17)	0.0710 (6)
N3	0.3595 (3)	−0.07569 (17)	0.08576 (17)	0.0646 (5)
C1	0.3443 (3)	0.00215 (19)	0.15970 (18)	0.0558 (5)
C2	0.4600 (3)	0.0087 (3)	0.2261 (2)	0.0691 (7)
H2	0.569 (4)	−0.039 (2)	0.230 (2)	0.083 (8)*
C3	0.2405 (3)	0.1382 (2)	0.25590 (18)	0.0612 (6)
C4	0.1251 (4)	0.2346 (3)	0.3018 (2)	0.0881 (8)
H4A	0.103783	0.299389	0.240158	0.132*
H4B	0.179996	0.257855	0.354842	0.132*
H4C	0.017095	0.208828	0.340157	0.132*
C5	0.0448 (3)	0.1185 (2)	0.1250 (2)	0.0619 (6)
H5A	−0.003 (3)	0.051 (2)	0.1289 (18)	0.063 (6)*
H5B	−0.040 (3)	0.1650 (19)	0.1716 (19)	0.062 (6)*
C6	0.0791 (3)	0.1848 (2)	0.0046 (2)	0.0604 (6)
H6A	0.170 (3)	0.141 (2)	−0.0427 (19)	0.065 (7)*
H6B	−0.029 (3)	0.204 (2)	−0.027 (2)	0.070 (7)*
C7	0.1776 (3)	0.3604 (2)	−0.0960 (2)	0.0584 (5)
C8	0.2397 (3)	0.46813 (19)	−0.0895 (2)	0.0578 (5)
C9	0.2958 (4)	0.5415 (2)	−0.1918 (3)	0.0776 (7)
H9	0.294 (3)	0.518 (2)	−0.264 (2)	0.080 (8)*
C10	0.3595 (4)	0.6420 (3)	−0.1898 (4)	0.0939 (10)
H10	0.397 (5)	0.693 (3)	−0.261 (3)	0.130 (12)*
C11	0.3661 (4)	0.6693 (3)	−0.0888 (4)	0.0907 (9)
H11	0.415 (4)	0.744 (3)	−0.091 (2)	0.104 (9)*
C12	0.3096 (3)	0.5983 (3)	0.0117 (3)	0.0803 (8)
H12	0.316 (4)	0.613 (2)	0.085 (3)	0.098 (9)*
C13	0.2470 (3)	0.4974 (2)	0.0121 (2)	0.0657 (6)
H13	0.210 (3)	0.448 (2)	0.081 (2)	0.075 (8)*
O1′	0.4959 (2)	0.15720 (18)	0.45717 (16)	0.0845 (6)
H1′	0.474 (4)	0.122 (3)	0.396 (3)	0.122 (11)*
O2′	0.7592 (3)	0.06517 (18)	0.41258 (17)	0.0914 (6)
N1′	1.0963 (3)	0.1476 (3)	0.6945 (2)	0.0842 (7)
H1′A	1.138 (4)	0.198 (3)	0.722 (3)	0.110 (11)*
H1′B	1.168 (4)	0.102 (3)	0.652 (3)	0.095 (10)*
C7′	0.6603 (3)	0.1271 (2)	0.4682 (2)	0.0643 (6)
C1′	0.7135 (3)	0.1792 (2)	0.55349 (18)	0.0617 (6)
C2′	0.6028 (4)	0.2643 (3)	0.6018 (2)	0.0823 (8)
H2′	0.478 (4)	0.298 (2)	0.574 (2)	0.103 (9)*
C3′	0.6603 (4)	0.3099 (3)	0.6800 (3)	0.0954 (10)
H3′	0.580 (4)	0.379 (3)	0.712 (3)	0.127 (11)*

C4′	0.8236 (4)	0.2728 (3)	0.7085 (3)	0.0847 (8)
H4′	0.872 (3)	0.309 (2)	0.762 (2)	0.093 (8)*
C5′	0.9352 (3)	0.1877 (2)	0.66121 (19)	0.0648 (6)
C6′	0.8774 (3)	0.1406 (2)	0.58364 (18)	0.0582 (5)
H6′	0.955 (3)	0.073 (2)	0.5552 (19)	0.068 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0721 (11)	0.0846 (13)	0.0996 (14)	0.0064 (10)	−0.0086 (10)	−0.0243 (11)
O2	0.0819 (12)	0.0795 (12)	0.0981 (13)	−0.0162 (9)	−0.0341 (10)	−0.0308 (10)
O3	0.0616 (9)	0.0565 (9)	0.0611 (9)	−0.0122 (7)	−0.0197 (7)	−0.0130 (7)
O4	0.1176 (15)	0.0857 (13)	0.0643 (11)	−0.0287 (11)	−0.0359 (10)	−0.0148 (9)
N1	0.0496 (10)	0.0614 (11)	0.0536 (10)	−0.0155 (8)	−0.0120 (8)	−0.0075 (8)
N2	0.0744 (13)	0.0885 (15)	0.0583 (12)	−0.0274 (11)	−0.0234 (10)	−0.0090 (11)
N3	0.0614 (12)	0.0627 (12)	0.0695 (12)	−0.0124 (10)	−0.0100 (10)	−0.0106 (10)
C1	0.0496 (12)	0.0627 (13)	0.0567 (12)	−0.0138 (10)	−0.0131 (9)	−0.0073 (10)
C2	0.0572 (14)	0.0846 (18)	0.0661 (15)	−0.0151 (13)	−0.0201 (12)	−0.0047 (13)
C3	0.0686 (14)	0.0683 (15)	0.0503 (12)	−0.0228 (12)	−0.0090 (11)	−0.0098 (11)
C4	0.105 (2)	0.093 (2)	0.0704 (17)	−0.0207 (17)	−0.0032 (15)	−0.0293 (15)
C5	0.0464 (12)	0.0662 (15)	0.0762 (16)	−0.0133 (11)	−0.0165 (11)	−0.0113 (13)
C6	0.0582 (13)	0.0589 (14)	0.0733 (15)	−0.0104 (11)	−0.0284 (12)	−0.0154 (12)
C7	0.0557 (12)	0.0619 (14)	0.0627 (14)	−0.0050 (10)	−0.0226 (10)	−0.0149 (11)
C8	0.0489 (11)	0.0547 (13)	0.0701 (15)	−0.0012 (9)	−0.0143 (10)	−0.0142 (11)
C9	0.0828 (18)	0.0676 (17)	0.0798 (18)	−0.0069 (13)	−0.0178 (14)	−0.0089 (14)
C10	0.092 (2)	0.0645 (18)	0.115 (3)	−0.0164 (15)	−0.0123 (19)	0.0019 (19)
C11	0.0734 (18)	0.0643 (18)	0.137 (3)	−0.0069 (14)	−0.0119 (18)	−0.032 (2)
C12	0.0664 (16)	0.0819 (19)	0.106 (2)	−0.0073 (14)	−0.0108 (15)	−0.0497 (18)
C13	0.0560 (13)	0.0693 (16)	0.0783 (17)	−0.0086 (11)	−0.0107 (12)	−0.0282 (14)
O1′	0.0754 (12)	0.1161 (15)	0.0759 (12)	−0.0193 (10)	−0.0249 (9)	−0.0324 (11)
O2′	0.0919 (13)	0.1102 (15)	0.0926 (13)	−0.0068 (11)	−0.0299 (11)	−0.0545 (12)
N1′	0.0798 (16)	0.0992 (18)	0.0921 (17)	−0.0008 (14)	−0.0358 (13)	−0.0468 (15)
C7′	0.0691 (15)	0.0757 (16)	0.0531 (13)	−0.0201 (12)	−0.0146 (11)	−0.0113 (12)
C1′	0.0692 (14)	0.0726 (15)	0.0482 (12)	−0.0178 (12)	−0.0107 (10)	−0.0153 (11)
C2′	0.0738 (17)	0.097 (2)	0.0850 (18)	0.0000 (15)	−0.0232 (14)	−0.0374 (16)
C3′	0.087 (2)	0.115 (2)	0.100 (2)	0.0085 (18)	−0.0258 (17)	−0.061 (2)
C4′	0.0858 (19)	0.100 (2)	0.0841 (19)	−0.0021 (16)	−0.0251 (15)	−0.0491 (17)
C5′	0.0704 (15)	0.0771 (16)	0.0535 (12)	−0.0120 (12)	−0.0150 (11)	−0.0209 (11)
C6′	0.0675 (14)	0.0623 (14)	0.0478 (12)	−0.0125 (11)	−0.0107 (10)	−0.0132 (10)

Geometric parameters (Å, º)

O1—N3	1.229 (3)	C9—C10	1.393 (4)
O2—N3	1.224 (2)	C10—H10	0.96 (4)
O3—C6	1.446 (3)	C10—C11	1.360 (5)
O3—C7	1.341 (3)	C11—H11	1.02 (3)
O4—C7	1.201 (3)	C11—C12	1.364 (5)
N1—C1	1.387 (3)	C12—H12	0.96 (3)

N1—C3	1.346 (3)	C12—C13	1.385 (4)
N1—C5	1.474 (3)	C13—H13	0.94 (3)
N2—C2	1.344 (3)	O1′—H1′	1.00 (4)
N2—C3	1.328 (3)	O1′—C7′	1.312 (3)
N3—C1	1.417 (3)	O2′—C7′	1.202 (3)
C1—C2	1.358 (3)	N1′—H1′A	0.90 (3)
C2—H2	0.95 (3)	N1′—H1′B	0.89 (3)
C3—C4	1.485 (4)	N1′—C5′	1.383 (3)
C4—H4A	0.9600	C7′—C1′	1.490 (3)
C4—H4B	0.9600	C1′—C2′	1.384 (4)
C4—H4C	0.9600	C1′—C6′	1.388 (3)
C5—H5A	0.95 (2)	C2′—H2′	1.08 (3)
C5—H5B	0.98 (2)	C2′—C3′	1.384 (4)
C5—C6	1.495 (3)	C3′—H3′	1.05 (3)
C6—H6A	0.99 (2)	C3′—C4′	1.374 (4)
C6—H6B	0.97 (2)	C4′—H4′	1.02 (3)
C7—C8	1.484 (3)	C4′—C5′	1.381 (4)
C8—C9	1.391 (4)	C5′—C6′	1.391 (3)
C8—C13	1.379 (3)	C6′—H6′	1.01 (2)
C9—H9	0.98 (3)		

C7—O3—C6	115.09 (17)	C8—C9—H9	118.2 (15)
C1—N1—C5	129.03 (19)	C8—C9—C10	119.7 (3)
C3—N1—C1	105.68 (18)	C10—C9—H9	122.1 (15)
C3—N1—C5	125.2 (2)	C9—C10—H10	119 (2)
C3—N2—C2	106.95 (19)	C11—C10—C9	120.5 (3)
O1—N3—C1	116.9 (2)	C11—C10—H10	121 (2)
O2—N3—O1	123.5 (2)	C10—C11—H11	117.9 (17)
O2—N3—C1	119.6 (2)	C10—C11—C12	120.1 (3)
N1—C1—N3	125.25 (18)	C12—C11—H11	122.0 (17)
C2—C1—N1	106.9 (2)	C11—C12—H12	122.7 (18)
C2—C1—N3	127.8 (2)	C11—C12—C13	120.6 (3)
N2—C2—C1	109.2 (2)	C13—C12—H12	116.7 (18)
N2—C2—H2	125.6 (16)	C8—C13—C12	120.2 (3)
C1—C2—H2	125.2 (16)	C8—C13—H13	119.1 (15)
N1—C3—C4	124.6 (2)	C12—C13—H13	120.7 (16)
N2—C3—N1	111.2 (2)	C7′—O1′—H1′	108.1 (19)
N2—C3—C4	124.2 (2)	H1′A—N1′—H1′B	120 (3)
C3—C4—H4A	109.5	C5′—N1′—H1′A	114 (2)
C3—C4—H4B	109.5	C5′—N1′—H1′B	115.7 (19)
C3—C4—H4C	109.5	O1′—C7′—C1′	113.7 (2)
H4A—C4—H4B	109.5	O2′—C7′—O1′	122.9 (2)
H4A—C4—H4C	109.5	O2′—C7′—C1′	123.3 (2)
H4B—C4—H4C	109.5	C2′—C1′—C7′	121.1 (2)
N1—C5—H5A	108.9 (13)	C2′—C1′—C6′	120.4 (2)
N1—C5—H5B	107.3 (13)	C6′—C1′—C7′	118.5 (2)
N1—C5—C6	112.39 (18)	C1′—C2′—H2′	120.0 (16)
H5A—C5—H5B	106.2 (19)	C1′—C2′—C3′	118.3 (3)

C6—C5—H5A	111.2 (13)	C3′—C2′—H2′	121.6 (16)
C6—C5—H5B	110.6 (13)	C2′—C3′—H3′	117.9 (19)
O3—C6—C5	107.92 (19)	C4′—C3′—C2′	121.2 (3)
O3—C6—H6A	108.7 (13)	C4′—C3′—H3′	120.7 (19)
O3—C6—H6B	108.6 (14)	C3′—C4′—H4′	122.7 (15)
C5—C6—H6A	111.5 (13)	C3′—C4′—C5′	121.1 (3)
C5—C6—H6B	108.9 (13)	C5′—C4′—H4′	116.1 (15)
H6A—C6—H6B	111.2 (19)	N1′—C5′—C6′	121.5 (2)
O3—C7—C8	113.10 (19)	C4′—C5′—N1′	120.5 (2)
O4—C7—O3	122.3 (2)	C4′—C5′—C6′	118.0 (2)
O4—C7—C8	124.6 (2)	C1′—C6′—C5′	121.0 (2)
C9—C8—C7	117.7 (2)	C1′—C6′—H6′	121.5 (13)
C13—C8—C7	123.3 (2)	C5′—C6′—H6′	117.4 (13)
C13—C8—C9	119.0 (2)		

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–salicylic acid (1/1) (bzmdslc)

Crystal data

$C_{13}H_{13}N_3O_4·C_7H_6O_3$
M_r = 413.38
Monoclinic, $P2_1/c$
a = 9.5055 (6) Å
b = 31.2239 (19) Å
c = 6.8578 (4) Å
β = 102.628 (2)°
V = 1986.2 (2) Å^3
Z = 4
$F(000)$ = 864
D_x = 1.382 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9833 reflections
θ = 2.6–27.4°
μ = 0.11 mm^{-1}
T = 301 K
Prismatic, colourless
0.68 × 0.24 × 0.16 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer
Multilayer mirrors monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.706, T_{max} = 0.746
69959 measured reflections
4553 independent reflections
3883 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 27.5°, θ_{min} = 2.9°
h = −12→12
k = −40→40
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.06
4553 reflections
347 parameters
100 restraints
Primary atom site location: dual
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 0.3493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.87803 (16)	0.63094 (4)	0.3909 (2)	0.0887 (4)
O2	0.92555 (13)	0.66308 (4)	0.67677 (19)	0.0803 (3)
O3	0.56700 (10)	0.71973 (3)	0.84768 (15)	0.0583 (2)
O4	0.64060 (13)	0.78754 (3)	0.84757 (19)	0.0771 (3)
N1	0.66295 (11)	0.63293 (3)	0.75126 (15)	0.0468 (2)
N2	0.52072 (13)	0.58617 (4)	0.56128 (18)	0.0598 (3)
N3	0.84921 (13)	0.64050 (4)	0.55066 (19)	0.0603 (3)
C1	0.54094 (14)	0.60942 (4)	0.7272 (2)	0.0536 (3)
C2	0.63221 (16)	0.59466 (4)	0.4743 (2)	0.0564 (3)
H2	0.6423 (17)	0.5809 (6)	0.355 (3)	0.073 (5)*
C3	0.71994 (14)	0.62349 (4)	0.58763 (18)	0.0480 (3)
C4	0.4412 (2)	0.60928 (8)	0.8662 (4)	0.0823 (5)
H4A	0.478 (3)	0.5934 (11)	0.988 (5)	0.159 (11)*
H4B	0.427 (3)	0.6365 (9)	0.916 (4)	0.135 (10)*
H4C	0.360 (4)	0.5953 (10)	0.805 (5)	0.156 (11)*
C5	0.72381 (16)	0.65981 (5)	0.92458 (19)	0.0558 (3)
H5A	0.8236 (17)	0.6512 (5)	0.969 (2)	0.058 (4)*
H5B	0.6706 (17)	0.6528 (5)	1.028 (2)	0.064 (4)*
C6	0.71571 (16)	0.70700 (5)	0.8807 (2)	0.0588 (3)
H6A	0.7540 (17)	0.7136 (5)	0.761 (3)	0.068 (4)*
C7	0.54390 (15)	0.76221 (4)	0.83503 (18)	0.0529 (3)
O1′	0.30972 (14)	0.53009 (4)	0.43561 (19)	0.0822 (4)
H1′	0.387 (2)	0.5478 (7)	0.473 (3)	0.102 (7)*
O2′	0.39947 (13)	0.51848 (4)	0.16738 (19)	0.0785 (3)
O3′	0.26597 (14)	0.46438 (4)	−0.10302 (19)	0.0787 (3)
H3′	0.333 (3)	0.4843 (7)	−0.043 (3)	0.105 (7)*
C7′	0.30950 (15)	0.51100 (4)	0.2653 (2)	0.0590 (3)
C1′	0.18997 (14)	0.48065 (4)	0.2017 (2)	0.0519 (3)
C2′	0.17227 (15)	0.45986 (4)	0.0179 (2)	0.0565 (3)
C3′	0.05451 (17)	0.43294 (5)	−0.0447 (3)	0.0659 (4)
H3′A	0.0427 (19)	0.4198 (6)	−0.172 (3)	0.080 (5)*
C4′	−0.04243 (17)	0.42646 (5)	0.0733 (3)	0.0686 (4)
H4′	−0.127 (2)	0.4075 (6)	0.022 (3)	0.085 (5)*
C5′	−0.02454 (16)	0.44612 (5)	0.2583 (3)	0.0668 (4)
H5′	−0.091 (2)	0.4411 (6)	0.340 (3)	0.088 (6)*
C6′	0.09104 (15)	0.47294 (5)	0.3210 (2)	0.0597 (3)
H6′	0.1065 (17)	0.4880 (5)	0.456 (3)	0.073 (5)*

C9	0.28162 (16)	0.74263 (5)	0.7797 (2)	0.0616 (3)
C10	0.1392 (2)	0.75472 (7)	0.7613 (3)	0.0787 (5)
C11	0.1046 (2)	0.79697 (7)	0.7762 (3)	0.0899 (6)
C12	0.2100 (3)	0.82743 (7)	0.8071 (3)	0.0932 (6)
C13	0.3531 (2)	0.81613 (5)	0.8229 (2)	0.0733 (4)
C8	0.38974 (16)	0.77321 (4)	0.81035 (17)	0.0544 (3)
H6B	0.7712 (18)	0.7223 (5)	0.994 (3)	0.069 (4)*
H13	0.4267 (19)	0.8361 (6)	0.839 (3)	0.072 (5)*
H9	0.3077 (18)	0.7123 (5)	0.771 (2)	0.070 (5)*
H12	0.190 (3)	0.8559 (8)	0.811 (4)	0.123 (8)*
H10	0.062 (3)	0.7333 (8)	0.741 (3)	0.112 (7)*
H11	0.000 (3)	0.8054 (7)	0.766 (3)	0.116 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1115 (10)	0.0842 (8)	0.0896 (8)	−0.0158 (7)	0.0642 (8)	−0.0120 (6)
O2	0.0697 (7)	0.0785 (7)	0.0976 (8)	−0.0226 (6)	0.0291 (6)	−0.0181 (6)
O3	0.0585 (5)	0.0463 (5)	0.0674 (6)	−0.0003 (4)	0.0077 (4)	−0.0079 (4)
O4	0.0822 (7)	0.0528 (6)	0.0979 (8)	−0.0125 (5)	0.0230 (6)	−0.0080 (5)
N1	0.0541 (6)	0.0414 (5)	0.0460 (5)	0.0006 (4)	0.0134 (4)	0.0012 (4)
N2	0.0613 (7)	0.0471 (6)	0.0695 (7)	−0.0066 (5)	0.0107 (5)	−0.0016 (5)
N3	0.0680 (7)	0.0500 (6)	0.0698 (7)	−0.0058 (5)	0.0300 (6)	−0.0020 (5)
C1	0.0541 (7)	0.0466 (6)	0.0614 (7)	−0.0008 (5)	0.0157 (6)	0.0071 (5)
C2	0.0697 (8)	0.0442 (6)	0.0557 (7)	−0.0018 (6)	0.0148 (6)	−0.0039 (5)
C3	0.0566 (7)	0.0405 (6)	0.0496 (6)	0.0001 (5)	0.0174 (5)	0.0016 (5)
C4	0.0773 (12)	0.0870 (13)	0.0938 (13)	−0.0075 (10)	0.0428 (10)	0.0071 (11)
C5	0.0621 (8)	0.0579 (8)	0.0451 (6)	0.0046 (6)	0.0070 (6)	−0.0045 (5)
C6	0.0568 (7)	0.0531 (7)	0.0638 (8)	−0.0014 (6)	0.0072 (6)	−0.0134 (6)
C7	0.0714 (8)	0.0457 (6)	0.0413 (6)	−0.0026 (6)	0.0116 (5)	−0.0068 (5)
O1′	0.0769 (7)	0.0870 (8)	0.0883 (8)	−0.0321 (6)	0.0302 (6)	−0.0276 (6)
O2′	0.0726 (7)	0.0773 (7)	0.0948 (8)	−0.0190 (6)	0.0387 (6)	−0.0027 (6)
O3′	0.0817 (8)	0.0850 (8)	0.0804 (7)	−0.0055 (6)	0.0414 (6)	−0.0145 (6)
C7′	0.0577 (7)	0.0500 (7)	0.0723 (9)	−0.0018 (6)	0.0211 (6)	0.0011 (6)
C1′	0.0501 (6)	0.0414 (6)	0.0664 (8)	0.0038 (5)	0.0177 (6)	0.0003 (5)
C2′	0.0573 (7)	0.0489 (7)	0.0672 (8)	0.0090 (5)	0.0224 (6)	−0.0005 (6)
C3′	0.0641 (8)	0.0579 (8)	0.0750 (10)	0.0052 (6)	0.0136 (7)	−0.0139 (7)
C4′	0.0542 (8)	0.0570 (8)	0.0942 (11)	−0.0026 (6)	0.0150 (7)	−0.0108 (8)
C5′	0.0552 (8)	0.0628 (9)	0.0882 (11)	−0.0045 (6)	0.0284 (7)	−0.0056 (7)
C6′	0.0575 (7)	0.0537 (7)	0.0728 (9)	−0.0007 (6)	0.0250 (6)	−0.0065 (6)
C9	0.0675 (8)	0.0617 (8)	0.0529 (7)	0.0029 (7)	0.0076 (6)	−0.0094 (6)
C10	0.0697 (10)	0.0947 (13)	0.0667 (9)	0.0059 (9)	0.0041 (8)	−0.0144 (8)
C11	0.0814 (12)	0.1051 (15)	0.0744 (11)	0.0296 (11)	−0.0021 (9)	−0.0137 (10)
C12	0.1147 (16)	0.0723 (11)	0.0852 (12)	0.0411 (11)	0.0056 (11)	−0.0024 (9)
C13	0.0964 (12)	0.0533 (8)	0.0661 (9)	0.0106 (8)	0.0089 (8)	−0.0010 (7)
C8	0.0739 (8)	0.0508 (7)	0.0363 (6)	0.0074 (6)	0.0077 (5)	−0.0034 (5)

Geometric parameters (Å, º)

O1—N3	1.2229 (16)	O2′—C7′	1.2196 (17)
O2—N3	1.2236 (16)	O3′—H3′	0.92 (2)
O3—C6	1.4378 (17)	O3′—C2′	1.3507 (17)
O3—C7	1.3441 (15)	C7′—C1′	1.4704 (19)
O4—C7	1.2015 (17)	C1′—C2′	1.3950 (19)
N1—C1	1.3518 (16)	C1′—C6′	1.3953 (19)
N1—C3	1.3803 (15)	C2′—C3′	1.391 (2)
N1—C5	1.4667 (16)	C3′—H3′A	0.951 (18)
N2—C1	1.3281 (18)	C3′—C4′	1.368 (2)
N2—C2	1.3509 (19)	C4′—H4′	1.001 (19)
N3—C3	1.4116 (17)	C4′—C5′	1.386 (2)
C1—C4	1.484 (2)	C5′—H5′	0.95 (2)
C2—H2	0.948 (17)	C5′—C6′	1.374 (2)
C2—C3	1.3514 (18)	C6′—H6′	1.019 (17)
C4—H4A	0.97 (3)	C9—C10	1.384 (2)
C4—H4B	0.94 (3)	C9—C8	1.385 (2)
C4—H4C	0.91 (3)	C9—H9	0.984 (17)
C5—H5A	0.969 (16)	C10—C11	1.369 (3)
C5—H5B	0.980 (16)	C10—H10	0.98 (2)
C5—C6	1.503 (2)	C11—C12	1.364 (3)
C6—H6A	0.988 (17)	C11—H11	1.02 (2)
C6—H6B	0.965 (17)	C12—C13	1.386 (3)
C7—C8	1.478 (2)	C12—H12	0.91 (2)
O1′—H1′	0.91 (2)	C13—C8	1.392 (2)
O1′—C7′	1.3111 (18)	C13—H13	0.925 (18)
C7—O3—C6	115.08 (11)	O1′—C7′—C1′	114.06 (12)
C1—N1—C3	105.29 (10)	O2′—C7′—O1′	122.59 (14)
C1—N1—C5	125.82 (11)	O2′—C7′—C1′	123.34 (14)
C3—N1—C5	128.73 (11)	C2′—C1′—C7′	120.02 (12)
C1—N2—C2	106.89 (11)	C2′—C1′—C6′	119.06 (12)
O1—N3—O2	124.02 (13)	C6′—C1′—C7′	120.90 (13)
O1—N3—C3	116.32 (12)	O3′—C2′—C1′	122.74 (13)
O2—N3—C3	119.66 (12)	O3′—C2′—C3′	117.89 (14)
N1—C1—C4	125.10 (15)	C3′—C2′—C1′	119.37 (13)
N2—C1—N1	111.15 (11)	C2′—C3′—H3′A	118.1 (11)
N2—C1—C4	123.75 (15)	C4′—C3′—C2′	120.49 (15)
N2—C2—H2	122.0 (10)	C4′—C3′—H3′A	121.4 (11)
N2—C2—C3	108.78 (12)	C3′—C4′—H4′	118.4 (11)
C3—C2—H2	129.2 (10)	C3′—C4′—C5′	120.82 (14)
N1—C3—N3	125.27 (11)	C5′—C4′—H4′	120.7 (11)
C2—C3—N1	107.88 (11)	C4′—C5′—H5′	120.2 (12)
C2—C3—N3	126.83 (12)	C6′—C5′—C4′	119.11 (15)
C1—C4—H4A	113.1 (19)	C6′—C5′—H5′	120.7 (12)
C1—C4—H4B	113.2 (17)	C1′—C6′—H6′	118.1 (9)
C1—C4—H4C	107.7 (19)	C5′—C6′—C1′	121.13 (14)

H4A—C4—H4B	102 (2)	C5′—C6′—H6′	120.8 (9)
H4A—C4—H4C	105 (2)	C10—C9—C8	120.28 (15)
H4B—C4—H4C	116 (3)	C10—C9—H9	120.7 (10)
N1—C5—H5A	106.3 (9)	C8—C9—H9	119.0 (10)
N1—C5—H5B	106.4 (9)	C9—C10—H10	121.0 (14)
N1—C5—C6	113.88 (11)	C11—C10—C9	120.15 (19)
H5A—C5—H5B	109.7 (13)	C11—C10—H10	118.8 (14)
C6—C5—H5A	109.7 (9)	C10—C11—H11	119.4 (13)
C6—C5—H5B	110.6 (9)	C12—C11—C10	120.21 (19)
O3—C6—C5	107.94 (12)	C12—C11—H11	120.3 (13)
O3—C6—H6A	109.8 (10)	C11—C12—C13	120.64 (18)
O3—C6—H6B	109.6 (10)	C11—C12—H12	122.2 (17)
C5—C6—H6A	111.0 (9)	C13—C12—H12	117.1 (17)
C5—C6—H6B	109.3 (10)	C12—C13—C8	119.65 (19)
H6A—C6—H6B	109.1 (13)	C12—C13—H13	122.8 (11)
O3—C7—C8	112.36 (11)	C8—C13—H13	117.5 (11)
O4—C7—O3	122.24 (13)	C9—C8—C7	122.78 (12)
O4—C7—C8	125.38 (12)	C9—C8—C13	119.05 (15)
C7′—O1′—H1′	111.8 (14)	C13—C8—C7	118.15 (14)
C2′—O3′—H3′	106.2 (14)		

1-[2-(Benzoyloxy)ethyl]-2-methyl-5-nitro-1*H*-imidazol-3-ium 3-carboxyprop-2-enoate (bzmdmlc)

Crystal data

$C_{13}H_{14}N_3O_4^+ \cdot C_4H_3O_4^-$
M_r = 391.33
Monoclinic, *C*2/*c*
a = 43.130 (3) Å
b = 5.7944 (4) Å
c = 15.2645 (11) Å
β = 109.600 (3)°
V = 3593.7 (5) Å^3
Z = 8
F(000) = 1632
D_x = 1.447 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 6422 reflections
θ = 2.7–26.1°
μ = 0.12 mm^{-1}
T = 302 K
Prism, clear light colourless
0.57 × 0.23 × 0.05 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer
Multilayer mirrors monochromator
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.261, T_{max} = 0.746
20803 measured reflections
4130 independent reflections
2159 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 27.5°, θ_{min} = 2.7°
h = −56→49
k = −7→7
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.147
S = 1.02
4130 reflections
322 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.8177P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}

$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0015 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.68004 (4)	0.6877 (3)	0.23662 (13)	0.0507 (5)
O1′	0.55288 (4)	−0.0276 (3)	0.21210 (14)	0.0618 (6)
O4	0.66174 (4)	0.3229 (3)	0.22612 (14)	0.0603 (5)
N1	0.61358 (4)	0.6620 (3)	0.25880 (13)	0.0390 (5)
N2	0.58882 (5)	0.3456 (4)	0.27408 (15)	0.0478 (5)
O3′	0.45356 (6)	0.2178 (3)	0.08155 (16)	0.0761 (6)
O2′	0.51306 (5)	0.2206 (3)	0.15210 (17)	0.0820 (7)
O4′	0.41448 (5)	−0.0382 (4)	0.03379 (16)	0.0823 (7)
O2	0.65266 (6)	0.9311 (4)	0.41184 (14)	0.0826 (7)
N3	0.64430 (5)	0.7380 (4)	0.42711 (17)	0.0569 (6)
O1	0.65247 (6)	0.6494 (4)	0.50428 (14)	0.0831 (7)
C3	0.62288 (6)	0.6050 (4)	0.35213 (17)	0.0421 (6)
C1	0.59273 (6)	0.4969 (4)	0.21254 (17)	0.0424 (6)
C8	0.71780 (6)	0.4014 (4)	0.31383 (17)	0.0434 (6)
C7	0.68393 (6)	0.4588 (4)	0.25489 (18)	0.0444 (6)
C5	0.62531 (7)	0.8476 (4)	0.2115 (2)	0.0442 (6)
C2	0.60735 (6)	0.4094 (4)	0.3611 (2)	0.0491 (7)
C6	0.64965 (7)	0.7620 (5)	0.1677 (2)	0.0495 (7)
C13	0.74353 (7)	0.5571 (5)	0.3278 (2)	0.0499 (7)
C1′	0.52336 (7)	0.0167 (4)	0.1699 (2)	0.0511 (7)
C2′	0.50025 (7)	−0.1817 (4)	0.1411 (2)	0.0532 (7)
C9	0.72408 (7)	0.1829 (4)	0.35499 (19)	0.0507 (7)
C4′	0.44353 (7)	0.0053 (5)	0.07005 (19)	0.0556 (7)
C3′	0.46770 (7)	−0.1857 (5)	0.1014 (2)	0.0543 (7)
C12	0.77498 (7)	0.4969 (5)	0.3810 (2)	0.0568 (7)
C11	0.78124 (8)	0.2810 (5)	0.4226 (2)	0.0587 (8)
C10	0.75578 (8)	0.1264 (5)	0.4091 (2)	0.0585 (8)
C4	0.57704 (9)	0.4779 (6)	0.1113 (2)	0.0587 (8)

H5A	0.6059 (6)	0.907 (4)	0.1597 (16)	0.045 (7)*
H13	0.7388 (6)	0.707 (4)	0.2973 (16)	0.052 (7)*
H5B	0.6357 (5)	0.968 (4)	0.2571 (16)	0.043 (7)*
H6A	0.6413 (6)	0.631 (5)	0.1212 (18)	0.063 (8)*
H2′	0.5118 (6)	−0.330 (4)	0.1577 (16)	0.055 (7)*
H2A	0.6072 (6)	0.328 (4)	0.4128 (17)	0.048 (7)*
H12	0.7929 (7)	0.609 (5)	0.3919 (18)	0.070 (9)*
H6B	0.6568 (6)	0.893 (5)	0.1377 (19)	0.067 (8)*
H10	0.7590 (6)	−0.031 (5)	0.4418 (19)	0.073 (9)*
H4A	0.5560 (9)	0.388 (6)	0.096 (2)	0.107 (12)*
H4B	0.5743 (8)	0.625 (6)	0.082 (2)	0.093 (11)*
H9	0.7040 (7)	0.076 (5)	0.3437 (19)	0.077 (9)*
H3′A	0.4572 (7)	−0.335 (5)	0.0881 (19)	0.073 (9)*
H2	0.5745 (8)	0.206 (5)	0.255 (2)	0.089 (10)*
H11	0.8042 (7)	0.243 (5)	0.4636 (19)	0.074 (9)*
H4C	0.5910 (8)	0.392 (6)	0.085 (2)	0.107 (13)*
H3′	0.4806 (11)	0.222 (6)	0.104 (3)	0.125 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0424 (10)	0.0375 (9)	0.0727 (12)	−0.0004 (8)	0.0200 (9)	0.0034 (8)
O1′	0.0417 (11)	0.0478 (11)	0.0899 (15)	−0.0047 (9)	0.0142 (10)	−0.0070 (10)
O4	0.0523 (11)	0.0405 (10)	0.0828 (14)	−0.0081 (9)	0.0158 (10)	−0.0015 (9)
N1	0.0381 (11)	0.0325 (10)	0.0461 (12)	−0.0026 (9)	0.0136 (10)	−0.0003 (9)
N2	0.0472 (13)	0.0411 (12)	0.0550 (14)	−0.0090 (10)	0.0171 (11)	−0.0029 (11)
O3′	0.0631 (14)	0.0454 (12)	0.1100 (18)	0.0084 (10)	0.0160 (13)	0.0107 (11)
O2′	0.0565 (13)	0.0390 (11)	0.140 (2)	−0.0027 (10)	0.0187 (14)	0.0045 (12)
O4′	0.0483 (13)	0.0800 (15)	0.1015 (17)	0.0036 (11)	0.0027 (12)	−0.0202 (13)
O2	0.0995 (17)	0.0666 (14)	0.0724 (15)	−0.0391 (13)	0.0165 (13)	−0.0087 (11)
N3	0.0533 (14)	0.0563 (14)	0.0560 (16)	−0.0119 (12)	0.0115 (12)	−0.0057 (12)
O1	0.0933 (17)	0.0892 (16)	0.0482 (13)	−0.0182 (13)	−0.0010 (12)	0.0089 (12)
C3	0.0391 (14)	0.0414 (13)	0.0442 (15)	−0.0025 (11)	0.0120 (12)	−0.0001 (11)
C1	0.0382 (13)	0.0389 (13)	0.0495 (16)	−0.0009 (11)	0.0139 (12)	−0.0009 (12)
C8	0.0455 (15)	0.0389 (13)	0.0502 (15)	−0.0023 (11)	0.0217 (13)	−0.0074 (11)
C7	0.0493 (16)	0.0345 (13)	0.0566 (16)	−0.0036 (12)	0.0273 (13)	−0.0049 (12)
C5	0.0449 (15)	0.0337 (13)	0.0541 (17)	−0.0012 (12)	0.0169 (14)	0.0069 (13)
C2	0.0500 (16)	0.0452 (15)	0.0514 (18)	−0.0066 (12)	0.0163 (14)	0.0037 (14)
C6	0.0489 (16)	0.0453 (15)	0.0570 (17)	−0.0004 (13)	0.0215 (14)	0.0077 (14)
C13	0.0472 (16)	0.0434 (15)	0.0611 (18)	−0.0022 (13)	0.0208 (14)	−0.0014 (13)
C1′	0.0471 (16)	0.0410 (15)	0.0672 (19)	−0.0036 (13)	0.0221 (14)	−0.0058 (13)
C2′	0.0520 (17)	0.0337 (13)	0.0702 (19)	−0.0014 (13)	0.0157 (15)	−0.0083 (13)
C9	0.0582 (18)	0.0403 (14)	0.0547 (17)	−0.0007 (14)	0.0205 (15)	−0.0046 (12)
C4′	0.0481 (17)	0.0578 (17)	0.0555 (18)	0.0052 (14)	0.0101 (14)	−0.0062 (14)
C3′	0.0491 (17)	0.0397 (15)	0.0679 (19)	−0.0043 (13)	0.0113 (14)	−0.0115 (13)
C12	0.0500 (17)	0.0546 (17)	0.068 (2)	−0.0046 (15)	0.0224 (15)	−0.0073 (15)
C11	0.0530 (18)	0.0646 (19)	0.0543 (18)	0.0110 (16)	0.0122 (15)	−0.0082 (15)
C10	0.071 (2)	0.0482 (16)	0.0541 (18)	0.0090 (16)	0.0189 (16)	−0.0020 (14)

C4	0.062 (2)	0.0612 (19)	0.0483 (18)	−0.0114 (17)	0.0126 (16)	−0.0067 (16)

Geometric parameters (Å, º)

O3—C7	1.354 (3)	C5—C6	1.505 (4)
O3—C6	1.444 (3)	C5—H5A	1.00 (2)
O1′—C1′	1.246 (3)	C5—H5B	0.98 (2)
O4—C7	1.202 (3)	C2—H2A	0.92 (2)
N1—C3	1.384 (3)	C6—H6A	1.02 (3)
N1—C1	1.340 (3)	C6—H6B	0.99 (3)
N1—C5	1.476 (3)	C13—C12	1.372 (4)
N2—C1	1.336 (3)	C13—H13	0.97 (2)
N2—C2	1.351 (3)	C1′—C2′	1.488 (3)
N2—H2	1.00 (3)	C2′—C3′	1.330 (4)
O3′—C4′	1.297 (3)	C2′—H2′	0.98 (2)
O3′—H3′	1.10 (4)	C9—C10	1.379 (4)
O2′—C1′	1.259 (3)	C9—H9	1.03 (3)
O2′—H3′	1.35 (4)	C4′—C3′	1.485 (4)
O4′—C4′	1.214 (3)	C3′—H3′A	0.97 (3)
O2—N3	1.222 (3)	C12—C11	1.388 (4)
N3—O1	1.223 (3)	C12—H12	0.98 (3)
N3—C3	1.431 (3)	C11—C10	1.378 (4)
C3—C2	1.347 (3)	C11—H11	1.00 (3)
C1—C4	1.469 (4)	C10—H10	1.02 (3)
C8—C7	1.474 (3)	C4—H4A	1.00 (4)
C8—C13	1.390 (3)	C4—H4B	0.95 (3)
C8—C9	1.399 (3)	C4—H4C	0.96 (3)
C7—O3—C6	117.5 (2)	C5—C6—H6A	114.8 (15)
C3—N1—C5	130.4 (2)	C5—C6—H6B	109.1 (15)
C1—N1—C3	106.48 (19)	H6A—C6—H6B	110 (2)
C1—N1—C5	122.8 (2)	C8—C13—H13	118.5 (14)
C1—N2—C2	109.8 (2)	C12—C13—C8	120.4 (3)
C1—N2—H2	122.4 (17)	C12—C13—H13	121.0 (15)
C2—N2—H2	127.8 (17)	O1′—C1′—O2′	122.0 (2)
C4′—O3′—H3′	109.5 (19)	O1′—C1′—C2′	117.4 (2)
C1′—O2′—H3′	110.5 (16)	O2′—C1′—C2′	120.6 (2)
O2—N3—O1	124.0 (2)	C1′—C2′—H2′	111.7 (14)
O2—N3—C3	119.5 (2)	C3′—C2′—C1′	130.4 (3)
O1—N3—C3	116.4 (2)	C3′—C2′—H2′	117.9 (14)
N1—C3—N3	125.5 (2)	C8—C9—H9	116.3 (15)
C2—C3—N1	108.8 (2)	C10—C9—C8	119.2 (3)
C2—C3—N3	125.6 (2)	C10—C9—H9	124.5 (15)
N1—C1—C4	126.8 (2)	O3′—C4′—C3′	119.8 (2)
N2—C1—N1	108.6 (2)	O4′—C4′—O3′	120.3 (3)
N2—C1—C4	124.6 (2)	O4′—C4′—C3′	119.8 (3)
C13—C8—C7	121.6 (2)	C2′—C3′—C4′	130.8 (3)
C13—C8—C9	119.6 (3)	C2′—C3′—H3′A	117.3 (17)

C9—C8—C7	118.8 (2)	C4′—C3′—H3′A	111.9 (17)
O3—C7—C8	112.0 (2)	C13—C12—C11	120.1 (3)
O4—C7—O3	122.5 (2)	C13—C12—H12	119.9 (16)
O4—C7—C8	125.4 (2)	C11—C12—H12	119.9 (16)
N1—C5—C6	112.4 (2)	C12—C11—H11	119.0 (16)
N1—C5—H5A	107.7 (13)	C10—C11—C12	119.6 (3)
N1—C5—H5B	108.7 (13)	C10—C11—H11	121.3 (16)
C6—C5—H5A	106.7 (13)	C9—C10—H10	116.6 (16)
C6—C5—H5B	109.2 (13)	C11—C10—C9	121.0 (3)
H5A—C5—H5B	112.1 (18)	C11—C10—H10	122.3 (15)
N2—C2—H2A	121.9 (15)	C1—C4—H4A	110.6 (19)
C3—C2—N2	106.3 (2)	C1—C4—H4B	111.2 (19)
C3—C2—H2A	131.7 (15)	C1—C4—H4C	110 (2)
O3—C6—C5	111.9 (2)	H4A—C4—H4B	113 (3)
O3—C6—H6A	107.9 (15)	H4A—C4—H4C	106 (3)
O3—C6—H6B	102.6 (15)	H4B—C4—H4C	106 (3)

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–isophthalic acid (1/1) (bzmdiac)

Crystal data

$C_{13}H_{13}N_3O_4{\cdot}C_8H_6O_4$
M_r = 441.39
Monoclinic, $P2_1/c$
a = 8.8300 (3) Å
b = 33.7182 (10) Å
c = 7.3199 (2) Å
β = 107.878 (1)°
V = 2074.13 (11) Å^3
Z = 4
$F(000)$ = 920
D_x = 1.414 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9928 reflections
θ = 2.4–30.4°
μ = 0.11 mm^{-1}
T = 304 K
Prism, clear light colourless
0.95 × 0.3 × 0.11 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer
Multilayer mirrors monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.649, T_{max} = 0.746
38842 measured reflections
6344 independent reflections
4809 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 30.5°, θ_{min} = 3.0°
h = −12→12
k = −48→48
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.145
S = 1.03
6344 reflections
365 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.4881P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.36882 (11)	0.28188 (3)	−0.12385 (16)	0.0549 (3)
O4′	1.31886 (13)	0.48005 (4)	0.42956 (16)	0.0617 (3)
O1′	0.78049 (13)	0.42754 (4)	0.32394 (16)	0.0610 (3)
O3′	1.47167 (13)	0.49211 (4)	0.72771 (17)	0.0697 (4)
N1	0.28442 (13)	0.36122 (3)	−0.03743 (16)	0.0452 (3)
O1	0.12528 (17)	0.37021 (4)	0.3517 (2)	0.0760 (4)
N2	0.48973 (15)	0.39681 (4)	0.13450 (19)	0.0537 (3)
N3	0.12377 (16)	0.36110 (4)	0.1893 (2)	0.0550 (3)
O2	0.01225 (15)	0.34423 (5)	0.0737 (2)	0.0833 (4)
O4	0.30372 (15)	0.21816 (4)	−0.1125 (3)	0.0846 (4)
O2′	0.68960 (17)	0.41614 (6)	0.5685 (2)	0.0982 (6)
C6′	1.07098 (15)	0.45287 (4)	0.5617 (2)	0.0431 (3)
C5′	1.21363 (15)	0.46743 (4)	0.68527 (19)	0.0438 (3)
C3	0.26003 (16)	0.37089 (4)	0.1350 (2)	0.0440 (3)
C8′	1.33969 (15)	0.48031 (4)	0.6041 (2)	0.0476 (3)
C1′	0.95064 (16)	0.44156 (4)	0.6348 (2)	0.0455 (3)
C8	0.56805 (17)	0.23453 (4)	−0.1057 (2)	0.0491 (3)
C1	0.42668 (17)	0.37765 (4)	−0.0295 (2)	0.0507 (3)
C2	0.38648 (18)	0.39278 (4)	0.2375 (2)	0.0509 (3)
C7	0.40177 (17)	0.24289 (5)	−0.1124 (2)	0.0526 (3)
C4′	1.23414 (18)	0.47070 (5)	0.8801 (2)	0.0522 (3)
C7′	0.79402 (18)	0.42688 (5)	0.5072 (2)	0.0539 (3)
C5	0.18737 (19)	0.33572 (5)	−0.1921 (2)	0.0544 (3)
C2′	0.97138 (19)	0.44485 (5)	0.8302 (2)	0.0552 (3)
C6	0.20736 (17)	0.29250 (5)	−0.1403 (3)	0.0539 (4)
C9	0.67651 (18)	0.26461 (5)	−0.0982 (3)	0.0578 (4)
C3′	1.1133 (2)	0.45954 (5)	0.9526 (2)	0.0585 (4)
C10	0.8293 (2)	0.25530 (6)	−0.0977 (3)	0.0664 (4)
C11	0.8741 (2)	0.21669 (6)	−0.1068 (3)	0.0664 (4)
C13	0.6152 (2)	0.19536 (5)	−0.1115 (3)	0.0669 (4)
C12	0.7681 (2)	0.18670 (6)	−0.1130 (3)	0.0739 (5)
C4	0.4995 (3)	0.37538 (8)	−0.1860 (4)	0.0781 (6)

H6′	1.0525 (19)	0.4509 (5)	0.425 (2)	0.049 (4)*
H5A	0.219 (2)	0.3419 (5)	−0.307 (3)	0.059 (5)*
H5B	0.077 (2)	0.3443 (5)	−0.217 (3)	0.060 (5)*
H6A	0.138 (2)	0.2775 (5)	−0.242 (3)	0.062 (5)*
H2	0.405 (2)	0.4048 (6)	0.365 (3)	0.066 (5)*
H4′	1.335 (2)	0.4810 (5)	0.964 (3)	0.059 (5)*
H6B	0.187 (2)	0.2868 (5)	−0.018 (3)	0.060 (5)*
H3′A	1.128 (2)	0.4626 (6)	1.089 (3)	0.072 (5)*
H9	0.645 (2)	0.2931 (6)	−0.091 (3)	0.076 (6)*
H13	0.538 (3)	0.1757 (7)	−0.116 (3)	0.083 (6)*
H2′	0.881 (2)	0.4366 (6)	0.884 (3)	0.074 (6)*
H1′	0.683 (3)	0.4171 (7)	0.249 (3)	0.099 (7)*
H11	0.983 (3)	0.2095 (6)	−0.109 (3)	0.084 (6)*
H10	0.906 (3)	0.2768 (6)	−0.092 (3)	0.080 (6)*
H12	0.796 (3)	0.1580 (7)	−0.126 (3)	0.091 (7)*
H4A	0.493 (4)	0.3484 (12)	−0.248 (5)	0.150 (12)*
H4B	0.598 (5)	0.3788 (12)	−0.136 (5)	0.154 (14)*
H3′	1.543 (4)	0.5032 (9)	0.655 (4)	0.125 (9)*
H4C	0.469 (5)	0.3945 (12)	−0.266 (6)	0.163 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0382 (5)	0.0566 (6)	0.0703 (7)	−0.0101 (4)	0.0171 (5)	−0.0127 (5)
O4′	0.0450 (5)	0.0863 (8)	0.0503 (6)	−0.0193 (5)	0.0093 (5)	−0.0118 (5)
O1′	0.0457 (5)	0.0788 (8)	0.0533 (6)	−0.0230 (5)	0.0073 (5)	−0.0005 (5)
O3′	0.0412 (5)	0.1084 (10)	0.0535 (6)	−0.0234 (6)	0.0055 (5)	−0.0159 (6)
N1	0.0418 (5)	0.0493 (6)	0.0435 (6)	−0.0070 (5)	0.0115 (4)	0.0015 (5)
O1	0.0815 (9)	0.0851 (9)	0.0766 (8)	−0.0039 (7)	0.0465 (7)	−0.0137 (7)
N2	0.0459 (6)	0.0519 (7)	0.0593 (7)	−0.0118 (5)	0.0102 (5)	0.0050 (5)
N3	0.0505 (7)	0.0522 (7)	0.0681 (8)	−0.0035 (5)	0.0269 (6)	−0.0042 (6)
O2	0.0555 (7)	0.1038 (10)	0.0973 (10)	−0.0306 (7)	0.0334 (7)	−0.0289 (8)
O4	0.0567 (7)	0.0643 (8)	0.1410 (13)	−0.0193 (6)	0.0427 (8)	−0.0104 (8)
O2′	0.0695 (8)	0.1590 (15)	0.0670 (8)	−0.0616 (9)	0.0225 (7)	−0.0070 (9)
C6′	0.0385 (6)	0.0428 (6)	0.0438 (7)	−0.0046 (5)	0.0067 (5)	−0.0041 (5)
C5′	0.0375 (6)	0.0416 (6)	0.0479 (7)	−0.0009 (5)	0.0067 (5)	−0.0034 (5)
C3	0.0405 (6)	0.0434 (6)	0.0481 (7)	−0.0028 (5)	0.0134 (5)	0.0009 (5)
C8′	0.0353 (6)	0.0517 (7)	0.0497 (7)	−0.0039 (5)	0.0041 (5)	−0.0087 (6)
C1′	0.0413 (6)	0.0425 (6)	0.0497 (7)	−0.0051 (5)	0.0092 (5)	−0.0002 (5)
C8	0.0444 (7)	0.0548 (8)	0.0476 (7)	−0.0079 (6)	0.0135 (6)	−0.0088 (6)
C1	0.0459 (7)	0.0529 (8)	0.0538 (8)	−0.0077 (6)	0.0162 (6)	0.0088 (6)
C2	0.0500 (7)	0.0476 (7)	0.0517 (8)	−0.0063 (6)	0.0104 (6)	−0.0012 (6)
C7	0.0454 (7)	0.0569 (8)	0.0566 (8)	−0.0129 (6)	0.0170 (6)	−0.0117 (6)
C4′	0.0453 (7)	0.0558 (8)	0.0486 (7)	−0.0023 (6)	0.0040 (6)	−0.0054 (6)
C7′	0.0463 (7)	0.0564 (8)	0.0570 (8)	−0.0159 (6)	0.0128 (6)	0.0003 (6)
C5	0.0444 (7)	0.0689 (9)	0.0445 (7)	−0.0055 (7)	0.0054 (6)	−0.0050 (6)
C2′	0.0510 (8)	0.0609 (9)	0.0536 (8)	−0.0032 (7)	0.0158 (7)	0.0033 (7)
C6	0.0353 (6)	0.0627 (9)	0.0614 (9)	−0.0116 (6)	0.0115 (6)	−0.0147 (7)

C9	0.0441 (7)	0.0587 (9)	0.0722 (10)	−0.0089 (6)	0.0201 (7)	−0.0106 (7)
C3′	0.0577 (9)	0.0701 (10)	0.0446 (7)	−0.0016 (7)	0.0111 (6)	−0.0018 (7)
C10	0.0454 (8)	0.0737 (11)	0.0820 (12)	−0.0092 (8)	0.0224 (8)	−0.0097 (9)
C11	0.0487 (8)	0.0821 (12)	0.0681 (10)	0.0060 (8)	0.0177 (8)	−0.0065 (9)
C13	0.0632 (10)	0.0555 (9)	0.0840 (12)	−0.0094 (8)	0.0254 (9)	−0.0075 (8)
C12	0.0688 (11)	0.0645 (11)	0.0887 (13)	0.0105 (9)	0.0250 (10)	−0.0045 (9)
C4	0.0825 (15)	0.0893 (15)	0.0776 (13)	−0.0158 (12)	0.0468 (12)	0.0077 (12)

Geometric parameters (Å, º)

O3—C7	1.3435 (19)	C8—C9	1.384 (2)
O3—C6	1.4388 (17)	C8—C13	1.389 (2)
O4′—C8′	1.2338 (18)	C1—C4	1.478 (3)
O1′—C7′	1.3101 (19)	C2—H2	0.983 (19)
O1′—H1′	0.93 (3)	C4′—C3′	1.382 (2)
O3′—C8′	1.2991 (16)	C4′—H4′	0.973 (19)
O3′—H3′	1.02 (3)	C5—C6	1.502 (2)
N1—C3	1.3829 (18)	C5—H5A	0.989 (18)
N1—C1	1.3578 (17)	C5—H5B	0.976 (18)
N1—C5	1.4694 (18)	C2′—C3′	1.389 (2)
O1—N3	1.2243 (18)	C2′—H2′	1.03 (2)
N2—C1	1.326 (2)	C6—H6A	0.952 (19)
N2—C2	1.357 (2)	C6—H6B	0.988 (18)
N3—O2	1.2236 (18)	C9—C10	1.384 (2)
N3—C3	1.4171 (18)	C9—H9	1.01 (2)
O4—C7	1.2019 (18)	C3′—H3′A	0.97 (2)
O2′—C7′	1.1986 (19)	C10—C11	1.368 (3)
C6′—C5′	1.3953 (18)	C10—H10	0.98 (2)
C6′—C1′	1.3821 (19)	C11—C12	1.369 (3)
C6′—H6′	0.968 (16)	C11—H11	1.00 (2)
C5′—C8′	1.479 (2)	C13—C12	1.385 (3)
C5′—C4′	1.386 (2)	C13—H13	0.94 (2)
C3—C2	1.3564 (19)	C12—H12	1.01 (2)
C1′—C7′	1.4955 (19)	C4—H4A	1.01 (4)
C1′—C2′	1.389 (2)	C4—H4B	0.84 (4)
C8—C7	1.481 (2)	C4—H4C	0.86 (4)
C7—O3—C6	116.03 (11)	O2′—C7′—O1′	123.34 (14)
C7′—O1′—H1′	111.7 (15)	O2′—C7′—C1′	122.45 (15)
C8′—O3′—H3′	108.4 (16)	N1—C5—C6	112.20 (13)
C3—N1—C5	128.58 (12)	N1—C5—H5A	106.5 (10)
C1—N1—C3	105.42 (11)	N1—C5—H5B	106.3 (10)
C1—N1—C5	125.80 (13)	C6—C5—H5A	112.2 (10)
C1—N2—C2	106.69 (12)	C6—C5—H5B	111.5 (10)
O1—N3—C3	117.19 (13)	H5A—C5—H5B	107.7 (15)
O2—N3—O1	123.67 (14)	C1′—C2′—H2′	120.0 (11)
O2—N3—C3	119.14 (13)	C3′—C2′—C1′	120.03 (15)
C5′—C6′—H6′	121.9 (10)	C3′—C2′—H2′	119.9 (11)

C1′—C6′—C5′	119.62 (13)	O3—C6—C5	107.41 (12)
C1′—C6′—H6′	118.5 (10)	O3—C6—H6A	108.6 (11)
C6′—C5′—C8′	118.94 (12)	O3—C6—H6B	109.3 (11)
C4′—C5′—C6′	120.14 (13)	C5—C6—H6A	108.8 (11)
C4′—C5′—C8′	120.90 (12)	C5—C6—H6B	112.1 (10)
N1—C3—N3	125.76 (12)	H6A—C6—H6B	110.6 (15)
C2—C3—N1	107.51 (12)	C8—C9—H9	120.0 (12)
C2—C3—N3	126.67 (13)	C10—C9—C8	119.72 (16)
O4′—C8′—O3′	122.69 (14)	C10—C9—H9	120.3 (12)
O4′—C8′—C5′	121.51 (12)	C4′—C3′—C2′	119.96 (15)
O3′—C8′—C5′	115.80 (13)	C4′—C3′—H3′A	119.1 (12)
C6′—C1′—C7′	121.54 (13)	C2′—C3′—H3′A	120.9 (12)
C6′—C1′—C2′	120.17 (13)	C9—C10—H10	119.3 (13)
C2′—C1′—C7′	118.26 (13)	C11—C10—C9	120.78 (17)
C9—C8—C7	121.91 (14)	C11—C10—H10	119.9 (13)
C9—C8—C13	119.19 (15)	C10—C11—C12	119.97 (17)
C13—C8—C7	118.88 (14)	C10—C11—H11	121.8 (12)
N1—C1—C4	124.24 (16)	C12—C11—H11	118.2 (12)
N2—C1—N1	111.31 (13)	C8—C13—H13	116.8 (13)
N2—C1—C4	124.42 (16)	C12—C13—C8	120.17 (17)
N2—C2—C3	109.07 (13)	C12—C13—H13	123.1 (13)
N2—C2—H2	122.9 (11)	C11—C12—C13	120.15 (18)
C3—C2—H2	128.1 (11)	C11—C12—H12	121.6 (13)
O3—C7—C8	112.45 (12)	C13—C12—H12	118.2 (13)
O4—C7—O3	122.45 (14)	C1—C4—H4A	114.7 (19)
O4—C7—C8	125.08 (15)	C1—C4—H4B	107 (2)
C5′—C4′—H4′	118.9 (10)	C1—C4—H4C	112 (3)
C3′—C4′—C5′	120.08 (14)	H4A—C4—H4B	103 (3)
C3′—C4′—H4′	121.1 (10)	H4A—C4—H4C	114 (3)
O1′—C7′—C1′	114.20 (12)	H4B—C4—H4C	105 (3)

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–resorcinol (2/1) (bzmdres)

Crystal data

$2C_{13}H_{13}N_3O_4{\cdot}C_6H_6O_2$
M_r = 660.63
Orthorhombic, *Pbca*
a = 26.3241 (4) Å
b = 7.1612 (1) Å
c = 33.8433 (5) Å
V = 6379.87 (16) Å^3
Z = 8
$F(000)$ = 2768
D_x = 1.376 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9896 reflections
θ = 3.1–68.2°
μ = 0.88 mm^{-1}
T = 300 K
Plate, clear light colourless
0.25 × 0.12 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.623, T_{max} = 0.753
121051 measured reflections
5865 independent reflections
4816 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

θ_{max} = 68.3°, θ_{min} = 2.6°
h = −31→31
k = −8→8
l = −40→40

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.147
S = 1.03
5865 reflections
540 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2 + 1.6636P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00043 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3B	0.29177 (5)	0.7763 (2)	0.21878 (3)	0.0676 (3)
O3A	0.70575 (5)	−0.1189 (2)	0.52879 (4)	0.0691 (3)
N1A	0.60485 (5)	−0.0111 (2)	0.55009 (4)	0.0594 (4)
N1B	0.39439 (5)	0.6490 (2)	0.19753 (4)	0.0606 (4)
O4B	0.21161 (6)	0.7410 (3)	0.19886 (5)	0.0946 (5)
N2A	0.55969 (6)	0.1485 (2)	0.50650 (5)	0.0698 (4)
O2′	0.52718 (8)	0.3814 (3)	0.44659 (5)	0.0978 (5)
O4A	0.78574 (6)	−0.1384 (3)	0.55011 (5)	0.1011 (6)
N2B	0.44240 (6)	0.5183 (3)	0.24363 (5)	0.0721 (4)
O1′	0.48855 (7)	0.5514 (3)	0.31647 (5)	0.1049 (6)
O2A	0.63071 (7)	0.1226 (3)	0.62598 (5)	0.1110 (6)
N3A	0.61124 (7)	0.2312 (3)	0.60258 (6)	0.0859 (5)
C8B	0.22773 (7)	0.8238 (2)	0.26590 (5)	0.0603 (4)
O2B	0.36980 (8)	0.4818 (4)	0.12448 (6)	0.1210 (7)
N3B	0.39162 (7)	0.3882 (3)	0.14929 (7)	0.0919 (6)
C8A	0.77042 (7)	−0.0609 (2)	0.48271 (5)	0.0616 (4)
C3A	0.59504 (6)	0.1642 (3)	0.56527 (5)	0.0629 (4)
O1A	0.60434 (8)	0.3983 (3)	0.60894 (7)	0.1274 (8)
C7B	0.24133 (7)	0.7746 (3)	0.22482 (5)	0.0637 (4)

C1B	0.41703 (7)	0.6707 (3)	0.23323 (5)	0.0633 (4)
C1A	0.58274 (7)	−0.0115 (3)	0.51389 (5)	0.0647 (4)
C7A	0.75635 (7)	−0.1104 (3)	0.52361 (5)	0.0660 (5)
C9A	0.73439 (8)	−0.0105 (3)	0.45482 (5)	0.0644 (4)
C3B	0.40651 (6)	0.4703 (3)	0.18565 (6)	0.0661 (5)
C2A	0.56744 (7)	0.2580 (3)	0.53836 (6)	0.0678 (5)
C6′	0.51323 (7)	0.3226 (3)	0.40973 (6)	0.0687 (5)
C2′	0.49229 (7)	0.4103 (3)	0.34347 (6)	0.0721 (5)
C9B	0.26411 (8)	0.8558 (3)	0.29468 (6)	0.0689 (5)
C1′	0.50863 (8)	0.4587 (3)	0.38117 (6)	0.0741 (5)
C2B	0.43581 (7)	0.3946 (3)	0.21394 (7)	0.0730 (5)
C3′	0.48105 (7)	0.2277 (3)	0.33438 (6)	0.0734 (5)
C5′	0.50283 (8)	0.1381 (3)	0.40091 (7)	0.0735 (5)
C6B	0.30779 (8)	0.7433 (4)	0.17856 (6)	0.0731 (5)
C5B	0.36357 (8)	0.7879 (3)	0.17681 (7)	0.0741 (5)
C5A	0.63229 (9)	−0.1684 (3)	0.56795 (7)	0.0777 (6)
C13B	0.17693 (8)	0.8428 (4)	0.27569 (7)	0.0797 (6)
C13A	0.82152 (8)	−0.0597 (3)	0.47209 (8)	0.0801 (6)
C10A	0.74957 (10)	0.0442 (3)	0.41755 (6)	0.0790 (6)
C4′	0.48680 (8)	0.0933 (3)	0.36331 (7)	0.0780 (5)
C10B	0.24940 (10)	0.9079 (3)	0.33226 (6)	0.0824 (6)
C6A	0.68875 (9)	−0.1410 (5)	0.56883 (6)	0.0838 (7)
C11B	0.19922 (10)	0.9302 (4)	0.34139 (7)	0.0853 (6)
O1B	0.40194 (8)	0.2250 (4)	0.14505 (9)	0.1469 (10)
C11A	0.79998 (11)	0.0491 (3)	0.40780 (8)	0.0891 (7)
C12A	0.83596 (10)	−0.0054 (4)	0.43460 (8)	0.0919 (7)
C4B	0.41432 (9)	0.8429 (4)	0.25758 (8)	0.0914 (7)
H4BA	0.436862	0.935305	0.246868	0.137*
H4BB	0.424152	0.814614	0.284228	0.137*
H4BC	0.380182	0.890062	0.257375	0.137*
C4A	0.58372 (10)	−0.1713 (4)	0.48615 (8)	0.0960 (7)
H4AA	0.617788	−0.218047	0.484027	0.144*
H4AB	0.572169	−0.131042	0.460625	0.144*
H4AC	0.561838	−0.268338	0.495797	0.144*
C12B	0.16312 (10)	0.8963 (4)	0.31324 (8)	0.0908 (7)
H3′	0.4671 (5)	0.1999 (19)	0.3050 (4)	0.036 (3)*
H5′	0.5072 (7)	0.034 (3)	0.4230 (5)	0.058 (5)*
H6BA	0.2885 (8)	0.827 (3)	0.1608 (7)	0.077 (6)*
H2A	0.5542 (9)	0.370 (4)	0.5409 (7)	0.081 (7)*
H9A	0.6979 (8)	−0.011 (3)	0.4627 (6)	0.075 (6)*
H1′A	0.5167 (8)	0.593 (3)	0.3891 (7)	0.081 (6)*
H13A	0.8432 (9)	−0.106 (3)	0.4913 (7)	0.082 (7)*
H4′	0.4801 (9)	−0.041 (4)	0.3582 (7)	0.090 (7)*
H5AA	0.6207 (10)	−0.178 (4)	0.5943 (9)	0.100 (8)*
H2B	0.4502 (9)	0.278 (4)	0.2145 (7)	0.093 (7)*
H9B	0.3015 (9)	0.846 (3)	0.2874 (7)	0.090 (7)*
H6BB	0.2999 (9)	0.602 (4)	0.1714 (7)	0.092 (7)*
H6AA	0.7045 (10)	−0.250 (4)	0.5801 (8)	0.103 (8)*

H5BA	0.3718 (9)	0.909 (3)	0.1898 (7)	0.084 (7)*
H11B	0.1864 (9)	0.985 (4)	0.3692 (8)	0.098 (7)*
H6AB	0.6966 (11)	−0.033 (4)	0.5822 (9)	0.103 (9)*
H13B	0.1530 (10)	0.809 (4)	0.2561 (8)	0.105 (8)*
H5BB	0.3746 (9)	0.788 (3)	0.1508 (8)	0.093 (7)*
H5AB	0.6241 (9)	−0.280 (4)	0.5517 (7)	0.086 (7)*
H11A	0.8124 (10)	0.095 (4)	0.3826 (9)	0.110 (9)*
H10A	0.7236 (10)	0.082 (4)	0.3987 (8)	0.103 (8)*
H10B	0.2797 (12)	0.934 (4)	0.3530 (9)	0.127 (10)*
H12B	0.1301 (11)	0.918 (4)	0.3203 (8)	0.109 (9)*
H12A	0.8730 (12)	−0.002 (4)	0.4288 (9)	0.124 (10)*
H1′	0.4698 (13)	0.507 (5)	0.2907 (11)	0.145 (12)*
H2′	0.5357 (15)	0.266 (6)	0.4639 (12)	0.174 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3B	0.0638 (7)	0.0860 (9)	0.0530 (6)	0.0111 (6)	−0.0044 (5)	0.0048 (6)
O3A	0.0637 (7)	0.0888 (9)	0.0549 (7)	0.0131 (6)	−0.0043 (5)	0.0036 (6)
N1A	0.0560 (7)	0.0656 (8)	0.0567 (8)	0.0012 (6)	0.0005 (6)	0.0059 (7)
N1B	0.0565 (8)	0.0702 (9)	0.0550 (8)	−0.0013 (7)	0.0003 (6)	0.0026 (7)
O4B	0.0744 (9)	0.1351 (14)	0.0744 (9)	0.0050 (9)	−0.0176 (7)	−0.0187 (9)
N2A	0.0701 (9)	0.0748 (10)	0.0646 (9)	0.0050 (8)	−0.0072 (7)	0.0050 (8)
O2′	0.1317 (14)	0.0893 (11)	0.0724 (9)	0.0065 (10)	−0.0237 (9)	0.0092 (8)
O4A	0.0755 (9)	0.1502 (16)	0.0777 (10)	0.0214 (10)	−0.0196 (8)	0.0123 (10)
N2B	0.0614 (8)	0.0855 (11)	0.0694 (9)	−0.0011 (8)	−0.0056 (7)	0.0111 (8)
O1′	0.1253 (14)	0.1048 (12)	0.0845 (10)	−0.0311 (10)	−0.0359 (10)	0.0347 (9)
O2A	0.0989 (12)	0.1692 (19)	0.0649 (9)	0.0149 (12)	−0.0146 (8)	−0.0071 (11)
N3A	0.0617 (9)	0.1170 (16)	0.0789 (11)	0.0060 (10)	−0.0095 (8)	−0.0261 (12)
C8B	0.0630 (9)	0.0559 (9)	0.0620 (9)	0.0073 (7)	−0.0047 (7)	0.0082 (8)
O2B	0.1083 (13)	0.177 (2)	0.0778 (10)	0.0200 (14)	−0.0198 (10)	−0.0295 (12)
N3B	0.0644 (10)	0.1138 (16)	0.0974 (14)	0.0070 (10)	−0.0029 (10)	−0.0408 (13)
C8A	0.0653 (10)	0.0546 (9)	0.0650 (10)	0.0009 (7)	−0.0032 (8)	−0.0134 (8)
C3A	0.0531 (9)	0.0731 (11)	0.0626 (10)	−0.0047 (8)	0.0008 (7)	−0.0051 (8)
O1A	0.1041 (13)	0.1358 (17)	0.1422 (18)	0.0224 (12)	−0.0328 (12)	−0.0735 (15)
C7B	0.0642 (10)	0.0633 (10)	0.0637 (10)	0.0086 (8)	−0.0112 (8)	0.0031 (8)
C1B	0.0574 (9)	0.0748 (11)	0.0578 (9)	−0.0063 (8)	0.0001 (7)	0.0008 (8)
C1A	0.0600 (9)	0.0712 (11)	0.0631 (10)	0.0022 (8)	−0.0023 (8)	−0.0012 (9)
C7A	0.0638 (10)	0.0679 (11)	0.0663 (10)	0.0121 (8)	−0.0102 (8)	−0.0054 (9)
C9A	0.0735 (11)	0.0595 (10)	0.0603 (10)	0.0014 (9)	−0.0032 (8)	−0.0057 (8)
C3B	0.0542 (9)	0.0754 (12)	0.0686 (11)	−0.0017 (8)	0.0020 (8)	−0.0090 (9)
C2A	0.0649 (10)	0.0597 (11)	0.0789 (12)	0.0006 (9)	−0.0028 (9)	0.0007 (9)
C6′	0.0618 (10)	0.0817 (13)	0.0626 (10)	0.0057 (9)	−0.0018 (8)	0.0095 (9)
C2′	0.0595 (10)	0.0903 (14)	0.0665 (11)	−0.0062 (9)	−0.0054 (8)	0.0188 (10)
C9B	0.0677 (11)	0.0771 (12)	0.0620 (10)	0.0084 (9)	−0.0060 (8)	0.0044 (9)
C1′	0.0758 (12)	0.0728 (12)	0.0737 (12)	−0.0028 (10)	−0.0119 (9)	0.0096 (10)
C2B	0.0590 (10)	0.0697 (12)	0.0901 (14)	0.0022 (9)	0.0012 (9)	0.0022 (11)
C3′	0.0629 (10)	0.0871 (14)	0.0702 (12)	−0.0060 (10)	0.0006 (9)	0.0015 (10)

C5′	0.0661 (11)	0.0772 (13)	0.0771 (12)	0.0032 (9)	0.0049 (9)	0.0168 (10)
C6B	0.0735 (11)	0.0950 (15)	0.0507 (9)	0.0169 (11)	−0.0042 (8)	0.0097 (10)
C5B	0.0786 (12)	0.0832 (14)	0.0604 (11)	0.0058 (10)	0.0039 (9)	0.0183 (10)
C5A	0.0805 (13)	0.0806 (14)	0.0720 (13)	0.0147 (11)	0.0060 (10)	0.0226 (11)
C13B	0.0654 (11)	0.0961 (15)	0.0777 (13)	0.0082 (11)	−0.0049 (10)	0.0039 (11)
C13A	0.0679 (11)	0.0853 (14)	0.0870 (15)	−0.0032 (10)	−0.0037 (11)	−0.0200 (12)
C10A	0.1019 (15)	0.0701 (12)	0.0649 (11)	−0.0068 (11)	−0.0003 (12)	−0.0053 (9)
C4′	0.0696 (12)	0.0771 (13)	0.0872 (14)	−0.0044 (10)	0.0064 (10)	0.0008 (11)
C10B	0.0908 (14)	0.0944 (15)	0.0621 (11)	0.0141 (12)	−0.0076 (11)	0.0014 (10)
C6A	0.0753 (13)	0.118 (2)	0.0580 (11)	0.0275 (13)	0.0007 (9)	0.0181 (13)
C11B	0.0988 (16)	0.0913 (15)	0.0657 (12)	0.0218 (12)	0.0088 (11)	0.0113 (11)
O1B	0.1119 (15)	0.1435 (19)	0.185 (2)	0.0282 (14)	−0.0336 (15)	−0.0900 (18)
C11A	0.1141 (19)	0.0790 (14)	0.0743 (14)	−0.0256 (13)	0.0189 (14)	−0.0207 (11)
C12A	0.0846 (15)	0.0949 (16)	0.0961 (17)	−0.0210 (13)	0.0233 (14)	−0.0306 (14)
C4B	0.0849 (14)	0.0990 (16)	0.0902 (15)	−0.0038 (12)	−0.0086 (12)	−0.0245 (13)
C4A	0.0959 (16)	0.0983 (17)	0.0939 (16)	0.0162 (13)	−0.0162 (13)	−0.0305 (14)
C12B	0.0744 (13)	0.1126 (19)	0.0853 (15)	0.0143 (13)	0.0163 (12)	0.0081 (13)

Geometric parameters (Å, º)

O3B—C7B	1.344 (2)	N3B—C3B	1.419 (3)
O3B—C6B	1.444 (2)	N3B—O1B	1.208 (3)
O3A—C7A	1.345 (2)	C8A—C7A	1.476 (3)
O3A—C6A	1.436 (2)	C8A—C9A	1.386 (3)
N1A—C3A	1.381 (2)	C8A—C13A	1.392 (3)
N1A—C1A	1.356 (2)	C3A—C2A	1.344 (3)
N1A—C5A	1.468 (2)	C1B—C4B	1.485 (3)
N1B—C1B	1.356 (2)	C1A—C4A	1.480 (3)
N1B—C3B	1.379 (3)	C9A—C10A	1.380 (3)
N1B—C5B	1.462 (3)	C3B—C2B	1.344 (3)
O4B—C7B	1.201 (2)	C6′—C1′	1.378 (3)
N2A—C1A	1.321 (3)	C6′—C5′	1.382 (3)
N2A—C2A	1.348 (3)	C2′—C1′	1.390 (3)
O2′—C6′	1.367 (3)	C2′—C3′	1.376 (3)
O4A—C7A	1.201 (2)	C9B—C10B	1.381 (3)
N2B—C1B	1.327 (3)	C3′—C4′	1.381 (3)
N2B—C2B	1.350 (3)	C5′—C4′	1.378 (3)
O1′—C2′	1.366 (3)	C6B—C5B	1.504 (3)
O2A—N3A	1.223 (3)	C5A—C6A	1.500 (3)
N3A—C3A	1.417 (3)	C13B—C12B	1.376 (3)
N3A—O1A	1.229 (3)	C13A—C12A	1.380 (4)
C8B—C7B	1.478 (3)	C10A—C11A	1.368 (4)
C8B—C9B	1.385 (3)	C10B—C11B	1.366 (3)
C8B—C13B	1.384 (3)	C11B—C12B	1.367 (4)
O2B—N3B	1.218 (3)	C11A—C12A	1.368 (4)
C7B—O3B—C6B	115.49 (14)	N2A—C1A—C4A	123.95 (18)
C7A—O3A—C6A	115.89 (15)	O3A—C7A—C8A	112.42 (15)

C3A—N1A—C5A	129.51 (17)	O4A—C7A—O3A	122.22 (19)
C1A—N1A—C3A	104.96 (15)	O4A—C7A—C8A	125.35 (19)
C1A—N1A—C5A	125.52 (18)	C10A—C9A—C8A	119.9 (2)
C1B—N1B—C3B	105.33 (15)	N1B—C3B—N3B	125.01 (19)
C1B—N1B—C5B	126.37 (17)	C2B—C3B—N1B	107.44 (18)
C3B—N1B—C5B	128.30 (17)	C2B—C3B—N3B	127.5 (2)
C1A—N2A—C2A	106.47 (16)	C3A—C2A—N2A	109.46 (18)
C1B—N2B—C2B	106.10 (16)	O2′—C6′—C1′	116.5 (2)
O2A—N3A—C3A	119.2 (2)	O2′—C6′—C5′	123.01 (18)
O2A—N3A—O1A	124.6 (2)	C1′—C6′—C5′	120.5 (2)
O1A—N3A—C3A	116.2 (2)	O1′—C2′—C1′	116.9 (2)
C9B—C8B—C7B	122.23 (17)	O1′—C2′—C3′	122.55 (19)
C13B—C8B—C7B	118.84 (17)	C3′—C2′—C1′	120.55 (19)
C13B—C8B—C9B	118.91 (19)	C10B—C9B—C8B	119.90 (19)
O2B—N3B—C3B	120.0 (2)	C6′—C1′—C2′	119.7 (2)
O1B—N3B—O2B	123.8 (2)	C3B—C2B—N2B	109.83 (19)
O1B—N3B—C3B	116.2 (2)	C2′—C3′—C4′	118.7 (2)
C9A—C8A—C7A	121.98 (17)	C4′—C5′—C6′	118.9 (2)
C9A—C8A—C13A	118.92 (19)	O3B—C6B—C5B	106.70 (17)
C13A—C8A—C7A	119.07 (18)	N1B—C5B—C6B	112.24 (17)
N1A—C3A—N3A	125.69 (18)	N1A—C5A—C6A	113.3 (2)
C2A—C3A—N1A	107.63 (17)	C12B—C13B—C8B	120.2 (2)
C2A—C3A—N3A	126.7 (2)	C12A—C13A—C8A	120.3 (2)
O3B—C7B—C8B	112.35 (15)	C11A—C10A—C9A	120.6 (2)
O4B—C7B—O3B	122.31 (18)	C5′—C4′—C3′	121.7 (2)
O4B—C7B—C8B	125.32 (18)	C11B—C10B—C9B	120.7 (2)
N1B—C1B—C4B	124.64 (18)	O3A—C6A—C5A	107.72 (18)
N2B—C1B—N1B	111.30 (17)	C10B—C11B—C12B	119.6 (2)
N2B—C1B—C4B	124.06 (18)	C10A—C11A—C12A	120.3 (2)
N1A—C1A—C4A	124.57 (18)	C11A—C12A—C13A	119.9 (2)
N2A—C1A—N1A	111.47 (17)	C11B—C12B—C13B	120.6 (2)

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–fumaric acid (2/1) (bzmdfma)

Crystal data

$C_{13}H_{13}N_3O_4{\cdot}0.5C_4H_4O_4$
M_r = 333.30
Monoclinic, $P2_1/c$
a = 9.0358 (5) Å
b = 26.6419 (14) Å
c = 6.8796 (3) Å
β = 102.419 (2)°
V = 1617.38 (14) Å^3
Z = 4

$F(000)$ = 696
D_x = 1.369 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9988 reflections
θ = 2.3–28.9°
μ = 0.11 mm^{-1}
T = 300 K
Prism, clear light colourless
0.63 × 0.17 × 0.17 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.620, T_{max} = 0.746
46849 measured reflections

3705 independent reflections
2625 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$

$h = -11 \rightarrow 11$
$k = -34 \rightarrow 34$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.151$
$S = 1.05$
3705 reflections
267 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.5999P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8887 (3)	0.59652 (9)	0.3299 (4)	0.1261 (9)
O2	0.9417 (2)	0.62892 (9)	0.6242 (4)	0.1134 (8)
O3	0.55707 (16)	0.70919 (5)	0.7641 (2)	0.0614 (4)
O4	0.6408 (2)	0.78808 (6)	0.7663 (3)	0.0818 (5)
N1	0.64502 (18)	0.60717 (6)	0.6676 (2)	0.0535 (4)
N2	0.4807 (2)	0.56134 (6)	0.4570 (3)	0.0640 (5)
N3	0.8562 (3)	0.60697 (8)	0.4893 (4)	0.0820 (6)
C1	0.5053 (2)	0.58656 (7)	0.6269 (3)	0.0574 (5)
C2	0.6064 (3)	0.56549 (8)	0.3829 (4)	0.0649 (6)
H2	0.620 (3)	0.5508 (9)	0.262 (4)	0.078 (7)*
C3	0.7094 (2)	0.59375 (7)	0.5099 (3)	0.0575 (5)
C4	0.3945 (3)	0.59055 (10)	0.7556 (4)	0.0838 (7)
H4A	0.417788	0.566096	0.860183	0.126*
H4B	0.294408	0.584567	0.677807	0.126*
H4C	0.399275	0.623576	0.812368	0.126*
C5	0.7116 (3)	0.63718 (9)	0.8440 (3)	0.0633 (5)
H5A	0.650 (3)	0.6299 (9)	0.940 (4)	0.069 (6)*

H5B	0.815 (3)	0.6255 (9)	0.896 (3)	0.073 (7)*
C6	0.7118 (2)	0.69224 (9)	0.7997 (4)	0.0651 (6)
H6A	0.766 (3)	0.7091 (9)	0.907 (4)	0.073 (7)*
H6B	0.751 (3)	0.6996 (9)	0.672 (4)	0.075 (7)*
C7	0.5365 (2)	0.75911 (8)	0.7537 (3)	0.0564 (5)
C8	0.3754 (2)	0.77333 (7)	0.7313 (3)	0.0540 (5)
C9	0.2606 (3)	0.73811 (9)	0.7113 (3)	0.0605 (5)
H9	0.287 (3)	0.7036 (10)	0.710 (4)	0.082 (8)*
C10	0.1132 (3)	0.75312 (10)	0.6989 (4)	0.0725 (6)
H10	0.031 (3)	0.7287 (10)	0.685 (4)	0.092 (8)*
C11	0.0794 (3)	0.80314 (11)	0.7083 (4)	0.0807 (7)
H11	−0.026 (3)	0.8135 (10)	0.702 (4)	0.087 (8)*
C12	0.1916 (4)	0.83847 (11)	0.7265 (4)	0.0856 (8)
H12	0.163 (3)	0.8738 (12)	0.734 (4)	0.101 (9)*
C13	0.3391 (3)	0.82380 (9)	0.7366 (4)	0.0717 (6)
H13	0.421 (3)	0.8472 (11)	0.743 (4)	0.094 (9)*
O1′	0.21422 (19)	0.52552 (7)	0.2699 (3)	0.0859 (6)
H1′	0.317 (4)	0.5368 (13)	0.342 (5)	0.121 (11)*
O2′	0.32943 (17)	0.49184 (7)	0.0484 (3)	0.0836 (5)
C1′	0.2163 (2)	0.50351 (7)	0.1006 (3)	0.0578 (5)
C2′	0.0625 (2)	0.49372 (8)	−0.0245 (4)	0.0629 (5)
H2′	0.055 (3)	0.4785 (11)	−0.152 (5)	0.102 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1359 (19)	0.1154 (17)	0.157 (2)	−0.0397 (14)	0.0970 (17)	−0.0559 (15)
O2	0.0673 (12)	0.1338 (18)	0.1422 (19)	−0.0313 (12)	0.0291 (12)	−0.0469 (15)
O3	0.0542 (8)	0.0556 (8)	0.0704 (9)	−0.0035 (6)	0.0045 (6)	−0.0106 (6)
O4	0.0761 (11)	0.0657 (10)	0.1059 (13)	−0.0188 (8)	0.0246 (9)	−0.0086 (9)
N1	0.0530 (9)	0.0500 (9)	0.0554 (9)	−0.0022 (7)	0.0070 (7)	−0.0012 (7)
N2	0.0587 (11)	0.0481 (9)	0.0776 (12)	−0.0030 (7)	−0.0020 (9)	0.0004 (8)
N3	0.0767 (14)	0.0666 (12)	0.1122 (17)	−0.0152 (10)	0.0416 (13)	−0.0255 (11)
C1	0.0508 (11)	0.0476 (10)	0.0712 (13)	−0.0010 (8)	0.0070 (9)	0.0084 (9)
C2	0.0772 (15)	0.0472 (11)	0.0676 (13)	−0.0024 (10)	0.0094 (11)	−0.0061 (9)
C3	0.0590 (12)	0.0471 (10)	0.0667 (12)	−0.0040 (8)	0.0147 (9)	−0.0041 (9)
C4	0.0685 (15)	0.0803 (16)	0.109 (2)	−0.0047 (12)	0.0329 (14)	0.0080 (14)
C5	0.0616 (13)	0.0701 (14)	0.0529 (11)	0.0021 (10)	0.0008 (10)	−0.0056 (10)
C6	0.0532 (12)	0.0675 (13)	0.0686 (14)	−0.0051 (10)	0.0000 (10)	−0.0185 (11)
C7	0.0679 (13)	0.0558 (11)	0.0450 (10)	−0.0084 (9)	0.0112 (9)	−0.0079 (8)
C8	0.0648 (12)	0.0562 (11)	0.0385 (9)	−0.0020 (9)	0.0058 (8)	−0.0047 (8)
C9	0.0643 (13)	0.0598 (13)	0.0535 (11)	−0.0015 (10)	0.0042 (9)	−0.0051 (9)
C10	0.0626 (14)	0.0813 (16)	0.0685 (14)	−0.0029 (12)	0.0027 (11)	−0.0098 (12)
C11	0.0717 (17)	0.0923 (19)	0.0706 (15)	0.0176 (15)	−0.0017 (12)	−0.0112 (13)
C12	0.092 (2)	0.0672 (16)	0.0907 (18)	0.0186 (14)	0.0038 (14)	−0.0066 (13)
C13	0.0855 (17)	0.0556 (13)	0.0709 (14)	−0.0021 (12)	0.0099 (12)	−0.0047 (10)
O1′	0.0529 (10)	0.0983 (13)	0.1000 (13)	−0.0022 (8)	0.0019 (8)	−0.0331 (10)
O2′	0.0461 (9)	0.1114 (14)	0.0934 (12)	0.0015 (8)	0.0152 (8)	−0.0062 (10)

C1′	0.0497 (11)	0.0496 (11)	0.0720 (13)	−0.0020 (8)	0.0085 (9)	−0.0015 (9)
C2′	0.0479 (11)	0.0601 (12)	0.0785 (14)	−0.0023 (9)	0.0083 (10)	−0.0123 (10)

Geometric parameters (Å, º)

O1—N3	1.227 (3)	C6—H6A	0.91 (3)
O2—N3	1.221 (3)	C6—H6B	1.03 (3)
O3—C6	1.439 (3)	C7—C8	1.480 (3)
O3—C7	1.343 (2)	C8—C9	1.383 (3)
O4—C7	1.206 (2)	C8—C13	1.386 (3)
N1—C1	1.350 (3)	C9—H9	0.95 (3)
N1—C3	1.384 (3)	C9—C10	1.375 (3)
N1—C5	1.469 (3)	C10—H10	0.98 (3)
N2—C1	1.325 (3)	C10—C11	1.372 (4)
N2—C2	1.346 (3)	C11—H11	0.98 (3)
N3—C3	1.408 (3)	C11—C12	1.369 (4)
C1—C4	1.475 (3)	C12—H12	0.98 (3)
C2—H2	0.95 (2)	C12—C13	1.376 (4)
C2—C3	1.359 (3)	C13—H13	0.96 (3)
C4—H4A	0.9600	O1′—H1′	1.00 (4)
C4—H4B	0.9600	O1′—C1′	1.308 (3)
C4—H4C	0.9600	O2′—C1′	1.195 (2)
C5—H5A	0.97 (2)	C1′—C2′	1.492 (3)
C5—H5B	0.98 (3)	C2′—C2′^{i}	1.290 (4)
C5—C6	1.498 (3)	C2′—H2′	0.96 (3)
C7—O3—C6	115.97 (16)	C5—C6—H6A	110.0 (15)
C1—N1—C3	105.33 (17)	C5—C6—H6B	112.0 (13)
C1—N1—C5	126.25 (19)	H6A—C6—H6B	112 (2)
C3—N1—C5	128.42 (18)	O3—C7—C8	112.38 (17)
C1—N2—C2	107.32 (18)	O4—C7—O3	122.2 (2)
O1—N3—C3	116.4 (2)	O4—C7—C8	125.4 (2)
O2—N3—O1	123.6 (2)	C9—C8—C7	122.44 (19)
O2—N3—C3	119.9 (2)	C9—C8—C13	118.9 (2)
N1—C1—C4	124.8 (2)	C13—C8—C7	118.6 (2)
N2—C1—N1	111.17 (19)	C8—C9—H9	118.1 (16)
N2—C1—C4	124.0 (2)	C10—C9—C8	120.3 (2)
N2—C2—H2	125.0 (15)	C10—C9—H9	121.5 (16)
N2—C2—C3	108.6 (2)	C9—C10—H10	121.3 (16)
C3—C2—H2	126.4 (15)	C11—C10—C9	120.1 (3)
N1—C3—N3	125.29 (19)	C11—C10—H10	118.5 (16)
C2—C3—N1	107.59 (19)	C10—C11—H11	119.7 (16)
C2—C3—N3	127.1 (2)	C12—C11—C10	120.3 (3)
C1—C4—H4A	109.5	C12—C11—H11	120.0 (16)
C1—C4—H4B	109.5	C11—C12—H12	117.6 (17)
C1—C4—H4C	109.5	C11—C12—C13	120.0 (3)
H4A—C4—H4B	109.5	C13—C12—H12	122.4 (17)
H4A—C4—H4C	109.5	C8—C13—H13	116.6 (17)

H4B—C4—H4C	109.5	C12—C13—C8	120.4 (2)
N1—C5—H5A	105.1 (14)	C12—C13—H13	123.0 (17)
N1—C5—H5B	108.7 (14)	C1′—O1′—H1′	112.7 (19)
N1—C5—C6	112.52 (18)	O1′—C1′—C2′	113.71 (19)
H5A—C5—H5B	109.2 (19)	O2′—C1′—O1′	124.1 (2)
C6—C5—H5A	111.0 (14)	O2′—C1′—C2′	122.2 (2)
C6—C5—H5B	110.2 (14)	C1′—C2′—H2′	118.3 (17)
O3—C6—C5	107.36 (19)	C2′^{i}—C2′—C1′	124.3 (3)
O3—C6—H6A	108.5 (15)	C2′^{i}—C2′—H2′	117.3 (17)
O3—C6—H6B	107.2 (14)		

Symmetry code: (i) −*x*, −*y*+1, −*z*.

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–malonic acid (2/1) (bzmdmln)

Crystal data

$2C_{13}H_{13}N_3O_4{\cdot}C_3H_2O_4$
M_r = 652.57
Orthorhombic, *Pbcn*
a = 26.1542 (4) Å
b = 7.2708 (1) Å
c = 16.6719 (3) Å
V = 3170.36 (9) Å^3
Z = 4
F(000) = 1360
D_x = 1.367 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 9937 reflections
θ = 3.1–72.5°
μ = 0.92 mm^{-1}
T = 300 K
Prism, clear light colourless
0.46 × 0.29 × 0.13 mm

Data collection

Bruker APEXII CCD diffractometer
φ and *ω* scans
Absorption correction: numerical (SADABS; Bruker, 2016)
T_{min} = 0.736, T_{max} = 0.907
54755 measured reflections
2893 independent reflections
2423 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 68.2°, θ_{min} = 5.6°
h = −31→31
k = −8→8
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.268
S = 1.13
2893 reflections
244 parameters
36 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1596P)^2 + 0.3629P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0039 (11)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O3	0.29519 (7)	0.6661 (3)	0.53894 (10)	0.1002 (6)	
O4	0.21543 (9)	0.6847 (4)	0.58610 (14)	0.1407 (10)	
N1	0.39769 (8)	0.5613 (3)	0.58207 (13)	0.0982 (6)	
C7	0.24416 (10)	0.6583 (4)	0.53037 (16)	0.0976 (7)	
N2	0.44070 (10)	0.3861 (5)	0.49826 (17)	0.1221 (9)	
C13	0.26247 (11)	0.5592 (3)	0.39102 (16)	0.0990 (7)	
H13	0.297280	0.557512	0.402389	0.119*	
N3	0.39562 (11)	0.3512 (5)	0.7007 (2)	0.1341 (10)	
C8	0.22811 (9)	0.6113 (3)	0.44877 (16)	0.0912 (7)	
O1	0.36955 (13)	0.4498 (6)	0.73879 (15)	0.1791 (15)	
C6	0.31291 (13)	0.6898 (5)	0.61932 (18)	0.1201 (10)	
H6A	0.304906	0.581714	0.651065	0.144*	
H6B	0.296435	0.795389	0.643718	0.144*	
C5	0.36982 (14)	0.7184 (5)	0.6162 (2)	0.1214 (10)	
H5A	0.377022	0.826914	0.584294	0.146*	
H5B	0.382282	0.741023	0.670087	0.146*	
C1	0.41726 (10)	0.5501 (5)	0.50779 (16)	0.1076 (9)	
C2	0.43619 (11)	0.2967 (5)	0.5682 (2)	0.1165 (9)	
H2	0.449468	0.180669	0.579041	0.140*	
C12	0.24521 (15)	0.5095 (5)	0.31615 (19)	0.1220 (10)	
H12	0.268778	0.474998	0.277171	0.146*	
C9	0.17676 (12)	0.6158 (5)	0.4293 (2)	0.1239 (10)	
H9	0.152766	0.653022	0.467173	0.149*	
O2	0.41029 (16)	0.2059 (6)	0.7247 (3)	0.2129 (19)	
C3	0.40976 (10)	0.3995 (4)	0.61981 (18)	0.1060 (8)	
C10	0.16136 (17)	0.5646 (7)	0.3534 (3)	0.1490 (15)	
H10	0.126798	0.568399	0.340365	0.179*	
C11	0.1952 (2)	0.5094 (6)	0.2979 (2)	0.1391 (13)	
H11	0.184141	0.471593	0.247515	0.167*	
C4	0.41453 (17)	0.6957 (7)	0.4471 (3)	0.1555 (16)	
H4A	0.380368	0.743804	0.445026	0.233*	
H4B	0.423554	0.646143	0.395651	0.233*	
H4C	0.437869	0.792578	0.460914	0.233*	
O1′	0.4899 (3)	0.1937 (13)	0.3802 (4)	0.138 (3)	0.5
H1′	0.462376	0.171352	0.401729	0.207*	0.5
C1′	0.4823 (3)	0.2427 (12)	0.3078 (5)	0.106 (2)	0.5
O2′	0.4576 (4)	0.3627 (13)	0.2891 (5)	0.213 (4)	0.5

C2′	0.500000	0.1017 (7)	0.250000	0.1213 (13)	
O2"	0.5116 (4)	0.1127 (9)	0.3942 (4)	0.152 (2)	0.5
C1"	0.4925 (3)	0.1738 (11)	0.3373 (6)	0.105 (2)	0.5
O1"	0.4611 (3)	0.3098 (12)	0.3421 (5)	0.185 (3)	0.5
H1"	0.450297	0.317907	0.388154	0.277*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0978 (12)	0.1145 (12)	0.0883 (11)	0.0141 (8)	0.0050 (8)	0.0030 (8)
O4	0.1174 (15)	0.190 (2)	0.1145 (16)	0.0319 (14)	0.0284 (12)	−0.0079 (15)
N1	0.0877 (12)	0.1129 (14)	0.0940 (13)	−0.0032 (10)	−0.0056 (9)	−0.0007 (10)
C7	0.0945 (15)	0.0968 (14)	0.1015 (16)	0.0193 (11)	0.0169 (12)	0.0104 (12)
N2	0.0934 (14)	0.160 (2)	0.1128 (17)	−0.0092 (14)	0.0132 (12)	−0.0241 (16)
C13	0.1102 (17)	0.0899 (14)	0.0968 (16)	−0.0003 (12)	0.0094 (12)	0.0096 (12)
N3	0.1095 (18)	0.169 (3)	0.124 (2)	0.0232 (17)	0.0120 (15)	0.0390 (19)
C8	0.0917 (14)	0.0806 (12)	0.1014 (15)	0.0051 (10)	0.0060 (11)	0.0209 (11)
O1	0.159 (2)	0.275 (4)	0.1037 (16)	0.063 (3)	0.0161 (15)	0.026 (2)
C6	0.120 (2)	0.150 (2)	0.0906 (16)	0.0267 (18)	−0.0044 (14)	−0.0155 (16)
C5	0.130 (2)	0.118 (2)	0.116 (2)	0.0064 (17)	−0.0114 (17)	−0.0212 (16)
C1	0.0871 (14)	0.141 (2)	0.0945 (16)	−0.0176 (14)	−0.0003 (11)	0.0035 (15)
C2	0.0947 (17)	0.124 (2)	0.131 (2)	−0.0053 (14)	0.0115 (16)	−0.0025 (17)
C12	0.151 (3)	0.1107 (19)	0.1046 (19)	−0.0162 (19)	0.0084 (19)	0.0106 (16)
C9	0.0969 (18)	0.140 (2)	0.135 (3)	0.0034 (16)	0.0031 (17)	0.025 (2)
O2	0.197 (3)	0.230 (4)	0.212 (4)	0.064 (3)	0.060 (3)	0.109 (3)
C3	0.0827 (14)	0.1249 (19)	0.1105 (18)	−0.0017 (13)	0.0031 (12)	0.0086 (15)
C10	0.126 (3)	0.165 (3)	0.157 (4)	−0.015 (2)	−0.040 (3)	0.038 (3)
C11	0.171 (3)	0.129 (2)	0.117 (2)	−0.039 (3)	−0.026 (2)	0.034 (2)
C4	0.131 (3)	0.207 (4)	0.128 (3)	−0.021 (3)	0.000 (2)	0.048 (3)
O1′	0.141 (5)	0.174 (6)	0.099 (4)	0.044 (4)	0.001 (3)	0.000 (4)
C1′	0.089 (4)	0.126 (6)	0.104 (4)	0.017 (4)	0.004 (3)	0.013 (4)
O2′	0.302 (10)	0.225 (7)	0.112 (4)	0.145 (7)	0.025 (5)	0.010 (5)
C2′	0.131 (3)	0.133 (3)	0.099 (3)	0.000	−0.001 (2)	0.000
O2"	0.210 (7)	0.134 (4)	0.111 (4)	0.034 (4)	−0.017 (4)	−0.010 (3)
C1"	0.079 (4)	0.099 (5)	0.135 (8)	0.003 (3)	0.015 (5)	0.010 (5)
O1"	0.203 (7)	0.218 (7)	0.134 (5)	0.106 (6)	0.029 (5)	0.018 (5)

Geometric parameters (Å, º)

O3—C7	1.344 (3)	C8—C9	1.382 (4)
O3—C6	1.428 (4)	C6—C5	1.504 (5)
O4—C7	1.210 (3)	C1—C4	1.466 (5)
N1—C5	1.469 (4)	C2—C3	1.333 (4)
N1—C1	1.343 (4)	C12—C11	1.344 (5)
N1—C3	1.371 (4)	C9—C10	1.380 (6)
C7—C8	1.464 (4)	C10—C11	1.341 (6)
N2—C1	1.350 (4)	O1′—C1′	1.274 (9)
N2—C2	1.340 (4)	C1′—O2′	1.129 (9)

C13—C8	1.370 (4)	C1′—C2′	1.482 (9)
C13—C12	1.376 (4)	C2′—C1"	1.559 (10)
N3—O1	1.176 (4)	C2′—C1"^{i}	1.559 (10)
N3—O2	1.193 (4)	O2"—C1"	1.161 (11)
N3—C3	1.441 (4)	C1"—O1"	1.288 (9)
C7—O3—C6	115.3 (2)	N2—C1—C4	125.4 (3)
C1—N1—C5	126.4 (3)	C3—C2—N2	109.6 (3)
C1—N1—C3	106.4 (2)	C11—C12—C13	121.7 (3)
C3—N1—C5	127.1 (3)	C10—C9—C8	119.5 (3)
O3—C7—C8	113.2 (2)	N1—C3—N3	125.4 (3)
O4—C7—O3	121.9 (3)	C2—C3—N1	107.7 (3)
O4—C7—C8	124.9 (3)	C2—C3—N3	126.9 (3)
C2—N2—C1	106.6 (3)	C11—C10—C9	121.4 (4)
C8—C13—C12	119.7 (3)	C10—C11—C12	119.1 (4)
O1—N3—O2	122.9 (4)	O1′—C1′—C2′	112.0 (7)
O1—N3—C3	120.4 (3)	O2′—C1′—O1′	124.5 (8)
O2—N3—C3	116.6 (4)	O2′—C1′—C2′	122.3 (7)
C13—C8—C7	122.0 (2)	C1′^{i}—C2′—C1′	92.4 (7)
C13—C8—C9	118.6 (3)	C1′^{i}—C2′—C1"^{i}	28.4 (3)
C9—C8—C7	119.4 (3)	C1′—C2′—C1"^{i}	114.4 (6)
O3—C6—C5	107.8 (3)	C1"^{i}—C2′—C1"	140.7 (7)
N1—C5—C6	113.4 (3)	O2"—C1"—C2′	125.5 (7)
N1—C1—N2	109.6 (3)	O2"—C1"—O1"	121.1 (10)
N1—C1—C4	125.0 (3)	O1"—C1"—C2′	113.4 (8)

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

1-[2-(Benzoyloxy)ethyl]-2-methyl-5-nitro-1*H*-imidazol-3-ium 2,6-dihydroxybenzoate (bzmd26dba)

Crystal data

$C_{13}H_{14}N_3O_4^+ \cdot C_7H_5O_4^-$
M_r = 429.38
Monoclinic, $P2_1/n$
a = 8.2443 (4) Å
b = 15.9009 (7) Å
c = 15.4526 (8) Å
β = 102.454 (2)°
V = 1978.04 (17) Å^3
Z = 4
$F(000)$ = 896
D_x = 1.442 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9886 reflections
θ = 2.5–27.5°
μ = 0.11 mm^{-1}
T = 301 K
Prism, clear light yellow
0.83 × 0.67 × 0.27 mm

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.490, T_{max} = 0.746
27674 measured reflections
4348 independent reflections
3408 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 27.5°, θ_{min} = 2.8°
h = −10→10
k = −20→20
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.185$
$S = 1.10$
4348 reflections
356 parameters
0 restraints

Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0913P)^2 + 0.5735P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O3	0.30908 (16)	0.45737 (9)	0.10470 (8)	0.0471 (3)
O1′	0.69550 (19)	0.38992 (10)	0.49968 (10)	0.0592 (4)
N1	0.25612 (18)	0.49805 (10)	0.28713 (10)	0.0407 (4)
O2	−0.08963 (19)	0.47761 (14)	0.24372 (12)	0.0777 (6)
O4′	1.0124 (2)	0.38277 (12)	0.56331 (14)	0.0725 (5)
O2′	0.5209 (2)	0.32169 (12)	0.56404 (14)	0.0728 (5)
N2	0.4226 (2)	0.44392 (10)	0.40318 (11)	0.0478 (4)
N3	−0.0133 (2)	0.44450 (12)	0.31200 (12)	0.0545 (5)
O1	−0.0783 (2)	0.40294 (14)	0.36109 (14)	0.0832 (6)
O4	0.1499 (2)	0.39405 (13)	−0.01207 (12)	0.0778 (6)
O3′	0.6249 (3)	0.22744 (13)	0.69473 (15)	0.0855 (6)
C1′	0.8096 (3)	0.30675 (11)	0.62457 (12)	0.0455 (4)
C1	0.4158 (2)	0.48952 (12)	0.33097 (13)	0.0441 (4)
C7′	0.6658 (3)	0.33991 (13)	0.55944 (13)	0.0485 (5)
C8	0.4427 (2)	0.37835 (12)	0.01068 (13)	0.0448 (4)
C6	0.1575 (2)	0.48994 (15)	0.12428 (14)	0.0494 (5)
C3	0.1624 (2)	0.45427 (12)	0.33634 (12)	0.0435 (4)
C2	0.2662 (3)	0.42133 (13)	0.40789 (13)	0.0487 (5)
C5	0.2007 (3)	0.54528 (13)	0.20416 (14)	0.0479 (5)
C2′	0.9742 (3)	0.32956 (13)	0.62356 (14)	0.0531 (5)
C7	0.2864 (2)	0.40967 (13)	0.03172 (13)	0.0484 (5)
C13	0.4327 (3)	0.33220 (15)	−0.06576 (17)	0.0618 (6)
C9	0.5971 (3)	0.39351 (15)	0.06467 (16)	0.0563 (5)

C3′	1.1037 (4)	0.29727 (17)	0.6877 (2)	0.0774 (8)
C4	0.5618 (3)	0.5256 (2)	0.3029 (2)	0.0649 (6)
C10	0.7374 (3)	0.36102 (18)	0.04179 (19)	0.0694 (7)
C12	0.5745 (4)	0.30044 (16)	−0.08794 (19)	0.0693 (7)
C6′	0.7806 (4)	0.25214 (13)	0.69090 (15)	0.0616 (6)
C11	0.7265 (3)	0.31502 (16)	−0.03340 (19)	0.0669 (6)
C4′	1.0704 (5)	0.24431 (17)	0.7517 (2)	0.0892 (11)
C5′	0.9118 (5)	0.22182 (16)	0.75427 (19)	0.0829 (9)
H5A	0.292 (3)	0.5844 (13)	0.2002 (14)	0.048 (5)*
H6A	0.086 (3)	0.4400 (15)	0.1351 (16)	0.058 (6)*
H2	0.238 (3)	0.3877 (14)	0.4495 (17)	0.058 (7)*
H5B	0.109 (3)	0.5774 (15)	0.2123 (15)	0.057 (6)*
H6B	0.099 (3)	0.5229 (15)	0.0737 (18)	0.065 (7)*
H12	0.564 (4)	0.2705 (17)	−0.142 (2)	0.081 (8)*
H9	0.599 (3)	0.4257 (16)	0.1141 (18)	0.063 (7)*
H3′	1.210 (4)	0.3103 (19)	0.676 (2)	0.088 (9)*
H11	0.823 (4)	0.2909 (16)	−0.0509 (18)	0.074 (8)*
H4′A	1.152 (4)	0.2196 (19)	0.798 (2)	0.095 (10)*
H4′	0.898 (5)	0.399 (2)	0.523 (2)	0.116 (12)*
H10	0.843 (4)	0.370 (2)	0.082 (2)	0.100 (10)*
H13	0.330 (4)	0.3231 (18)	−0.103 (2)	0.086 (9)*
H5′	0.879 (4)	0.187 (2)	0.801 (2)	0.102 (10)*
H2′	0.562 (5)	0.270 (3)	0.638 (3)	0.133 (14)*
H1′	0.548 (6)	0.415 (2)	0.454 (3)	0.132 (13)*
H4A	0.575 (5)	0.504 (2)	0.250 (3)	0.117 (13)*
H4B	0.554 (6)	0.585 (3)	0.303 (3)	0.133 (15)*
H4C	0.653 (6)	0.515 (3)	0.347 (3)	0.138 (15)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0316 (7)	0.0630 (8)	0.0445 (7)	0.0046 (6)	0.0037 (5)	−0.0008 (6)
O1′	0.0422 (8)	0.0778 (10)	0.0546 (8)	0.0077 (7)	0.0037 (6)	0.0114 (7)
N1	0.0297 (8)	0.0472 (8)	0.0446 (8)	0.0045 (6)	0.0068 (6)	−0.0010 (6)
O2	0.0341 (8)	0.1341 (16)	0.0631 (10)	0.0079 (9)	0.0061 (7)	0.0170 (10)
O4′	0.0427 (9)	0.0877 (12)	0.0845 (12)	−0.0045 (8)	0.0080 (8)	0.0172 (9)
O2′	0.0443 (9)	0.0815 (11)	0.0917 (13)	−0.0026 (8)	0.0130 (8)	0.0032 (10)
N2	0.0387 (9)	0.0542 (9)	0.0468 (9)	0.0072 (7)	0.0006 (7)	−0.0072 (7)
N3	0.0333 (9)	0.0752 (12)	0.0560 (10)	0.0015 (8)	0.0114 (7)	0.0005 (8)
O1	0.0479 (10)	0.1147 (15)	0.0903 (13)	−0.0120 (10)	0.0222 (9)	0.0255 (11)
O4	0.0375 (9)	0.1101 (14)	0.0769 (11)	0.0044 (8)	−0.0073 (8)	−0.0305 (10)
O3′	0.0927 (16)	0.0810 (12)	0.0888 (14)	−0.0202 (11)	0.0326 (12)	0.0109 (11)
C1′	0.0491 (11)	0.0408 (9)	0.0442 (9)	0.0021 (8)	0.0048 (8)	−0.0074 (7)
C1	0.0318 (9)	0.0482 (10)	0.0511 (10)	0.0044 (7)	0.0061 (7)	−0.0099 (8)
C7′	0.0411 (11)	0.0518 (10)	0.0517 (11)	0.0025 (8)	0.0078 (8)	−0.0100 (8)
C8	0.0391 (10)	0.0469 (9)	0.0474 (10)	0.0003 (8)	0.0071 (8)	0.0036 (8)
C6	0.0315 (10)	0.0673 (13)	0.0481 (10)	0.0081 (9)	0.0057 (8)	0.0033 (9)
C3	0.0339 (10)	0.0502 (10)	0.0461 (9)	0.0032 (7)	0.0076 (7)	−0.0035 (8)

C2	0.0459 (11)	0.0546 (11)	0.0445 (10)	0.0032 (9)	0.0075 (8)	−0.0003 (8)
C5	0.0411 (11)	0.0499 (10)	0.0532 (11)	0.0095 (9)	0.0110 (8)	0.0076 (8)
C2′	0.0481 (12)	0.0484 (10)	0.0569 (11)	0.0023 (8)	−0.0017 (9)	−0.0042 (9)
C7	0.0371 (10)	0.0581 (11)	0.0472 (10)	0.0012 (8)	0.0026 (8)	0.0017 (8)
C13	0.0543 (14)	0.0662 (14)	0.0628 (13)	−0.0018 (11)	0.0084 (11)	−0.0111 (11)
C9	0.0408 (11)	0.0693 (13)	0.0559 (12)	0.0008 (9)	0.0040 (9)	−0.0047 (10)
C3′	0.0580 (16)	0.0624 (14)	0.0941 (19)	0.0003 (12)	−0.0227 (14)	−0.0016 (13)
C4	0.0343 (12)	0.0828 (18)	0.0783 (17)	−0.0058 (11)	0.0140 (11)	−0.0068 (14)
C10	0.0387 (13)	0.0857 (17)	0.0824 (17)	0.0056 (11)	0.0097 (11)	−0.0019 (14)
C12	0.0786 (18)	0.0628 (14)	0.0718 (15)	0.0038 (12)	0.0281 (13)	−0.0111 (12)
C6′	0.0806 (17)	0.0450 (10)	0.0571 (12)	−0.0043 (10)	0.0104 (11)	−0.0039 (9)
C11	0.0559 (15)	0.0649 (14)	0.0858 (17)	0.0122 (11)	0.0286 (13)	0.0062 (12)
C4′	0.106 (3)	0.0537 (14)	0.0816 (18)	0.0071 (14)	−0.0370 (17)	0.0058 (13)
C5′	0.117 (3)	0.0514 (13)	0.0667 (15)	−0.0072 (14)	−0.0101 (16)	0.0113 (12)

Geometric parameters (Å, º)

O3—C6	1.444 (2)	C6—C5	1.495 (3)
O3—C7	1.338 (2)	C6—H6A	1.02 (2)
O1′—C7′	1.282 (3)	C6—H6B	0.98 (3)
O1′—H1′	1.32 (5)	C3—C2	1.350 (3)
N1—C1	1.351 (2)	C2—H2	0.90 (2)
N1—C3	1.383 (2)	C5—H5A	0.99 (2)
N1—C5	1.471 (2)	C5—H5B	0.95 (2)
O2—N3	1.225 (2)	C2′—C3′	1.389 (3)
O4′—C2′	1.345 (3)	C13—C12	1.383 (4)
O4′—H4′	1.05 (4)	C13—H13	0.93 (3)
O2′—C7′	1.246 (3)	C9—C10	1.381 (3)
O2′—H2′	1.38 (5)	C9—H9	0.92 (3)
N2—C1	1.322 (3)	C3′—C4′	1.371 (5)
N2—C2	1.355 (3)	C3′—H3′	0.96 (3)
N2—H1′	1.25 (5)	C4—H4A	0.92 (4)
N3—O1	1.214 (2)	C4—H4B	0.95 (4)
N3—C3	1.424 (3)	C4—H4C	0.92 (5)
O4—C7	1.207 (3)	C10—C11	1.359 (4)
O3′—C6′	1.356 (3)	C10—H10	0.97 (4)
O3′—H2′	1.15 (5)	C12—C11	1.370 (4)
C1′—C7′	1.477 (3)	C12—H12	0.94 (3)
C1′—C2′	1.408 (3)	C6′—C5′	1.380 (4)
C1′—C6′	1.402 (3)	C11—H11	0.97 (3)
C1—C4	1.480 (3)	C4′—C5′	1.365 (5)
C8—C7	1.481 (3)	C4′—H4′A	0.96 (4)
C8—C13	1.378 (3)	C5′—H5′	1.00 (3)
C8—C9	1.385 (3)		

C7—O3—C6	114.21 (15)	C6—C5—H5B	111.8 (15)
C7′—O1′—H1′	105.9 (17)	H5A—C5—H5B	108.1 (19)
C1—N1—C3	105.86 (15)	O4′—C2′—C1′	122.70 (19)

C1—N1—C5	125.05 (17)	O4′—C2′—C3′	117.9 (2)
C3—N1—C5	129.09 (16)	C3′—C2′—C1′	119.4 (2)
C2′—O4′—H4′	104.8 (19)	O3—C7—C8	113.92 (17)
C7′—O2′—H2′	96.7 (17)	O4—C7—O3	122.18 (19)
C1—N2—C2	108.84 (17)	O4—C7—C8	123.90 (19)
C1—N2—H1′	127.8 (19)	C8—C13—C12	120.6 (2)
C2—N2—H1′	122.7 (18)	C8—C13—H13	119.3 (19)
O2—N3—C3	119.01 (18)	C12—C13—H13	120.0 (19)
O1—N3—O2	123.94 (19)	C8—C9—H9	116.6 (17)
O1—N3—C3	117.05 (18)	C10—C9—C8	119.5 (2)
C6′—O3′—H2′	94 (2)	C10—C9—H9	123.9 (17)
C2′—C1′—C7′	122.29 (19)	C2′—C3′—H3′	112 (2)
C6′—C1′—C7′	118.7 (2)	C4′—C3′—C2′	119.9 (3)
C6′—C1′—C2′	118.9 (2)	C4′—C3′—H3′	127.4 (19)
N1—C1—C4	125.5 (2)	C1—C4—H4A	112 (2)
N2—C1—N1	109.75 (17)	C1—C4—H4B	109 (3)
N2—C1—C4	124.8 (2)	C1—C4—H4C	107 (3)
O1′—C7′—C1′	117.54 (18)	H4A—C4—H4B	113 (4)
O2′—C7′—O1′	121.3 (2)	H4A—C4—H4C	111 (4)
O2′—C7′—C1′	121.1 (2)	H4B—C4—H4C	104 (4)
C13—C8—C7	118.26 (19)	C9—C10—H10	118 (2)
C13—C8—C9	119.1 (2)	C11—C10—C9	121.0 (2)
C9—C8—C7	122.66 (19)	C11—C10—H10	121 (2)
O3—C6—C5	108.75 (16)	C13—C12—H12	118.5 (19)
O3—C6—H6A	108.1 (13)	C11—C12—C13	119.7 (2)
O3—C6—H6B	108.8 (15)	C11—C12—H12	121.8 (19)
C5—C6—H6A	111.4 (13)	O3′—C6′—C1′	121.5 (2)
C5—C6—H6B	109.4 (14)	O3′—C6′—C5′	118.2 (3)
H6A—C6—H6B	110 (2)	C5′—C6′—C1′	120.3 (3)
N1—C3—N3	124.52 (17)	C10—C11—C12	120.0 (2)
C2—C3—N1	108.34 (17)	C10—C11—H11	122.8 (17)
C2—C3—N3	127.11 (19)	C12—C11—H11	117.2 (17)
N2—C2—H2	125.8 (17)	C3′—C4′—H4′A	126 (2)
C3—C2—N2	107.21 (19)	C5′—C4′—C3′	121.6 (3)
C3—C2—H2	126.8 (17)	C5′—C4′—H4′A	113 (2)
N1—C5—C6	113.14 (17)	C6′—C5′—H5′	115 (2)
N1—C5—H5A	106.2 (13)	C4′—C5′—C6′	119.8 (3)
N1—C5—H5B	105.5 (14)	C4′—C5′—H5′	126 (2)
C6—C5—H5A	111.6 (13)		

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl benzoate–3,5-dihydroxybenzoic acid (3/1) (bzmd35dba)

Crystal data

$3C_{13}H_{13}N_3O_4·C_7H_6O_4$
M_r = 979.91
Monoclinic, $P2_1/n$
a = 7.1481 (2) Å
b = 36.7892 (8) Å
c = 18.0584 (4) Å
β = 100.451 (1)°
V = 4670.1 (2) Å^3
Z = 4
$F(000)$ = 2048
D_x = 1.394 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å

Cell parameters from 9896 reflections
θ = 3.5–67.6°
μ = 0.91 mm^{-1}

T = 300 K
Prism, clear light colourless
0.28 × 0.14 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Multilayer mirrors monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.835, T_{max} = 0.986
56516 measured reflections

8547 independent reflections
5499 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 68.7°, θ_{min} = 2.8°
h = −7→8
k = −44→44
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.176
S = 1.01
8547 reflections
844 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0833P)^2 + 2.1514P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00125 (13)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Single-crystal X-ray diffraction data collection (scans and ω scans with κ and θ offsets) were performed at room temperature on a Bruker AXS D8 VENTURE equipped with a Kappa goniometer, PHOTON II CPAD detector, a Mo $K\alpha$ INCOATEC IμS 3.0 microfocus source (λ = 0.71073 Å). The crystal centring, unit-cell determination, refinement of the unit-cell parameters and data collection was controlled through the program *APEX3* (Bruker, 2012). The frame integration was performed using *SAINT* (Bruker, 2016) and the intensities were scaled and absorption corrected using *SADABS* (Bruker, 2001). Using *OLEX2* (Dolomanov *et al.*, 2009), the structure was solved by intrinsic phasing using *SHELXT* (Sheldrick, 2015) and refined by full-matrix least-squares calculation based on F^2 for all reflection using *SHELXL* (Sheldrick, 2007). All non-H atoms were refined anisotropically.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1C	0.8254 (4)	0.36199 (7)	−0.06761 (14)	0.0939 (7)	
O2C	0.5826 (4)	0.32866 (7)	−0.11345 (12)	0.0874 (7)	
O3C	0.3392 (3)	0.26359 (5)	0.03750 (10)	0.0688 (5)	
O3A	0.7853 (3)	0.47087 (5)	0.86671 (10)	0.0634 (5)	
N1A	0.9537 (3)	0.51097 (6)	0.74799 (11)	0.0540 (5)	
O3B	0.7069 (3)	0.71873 (5)	0.49400 (11)	0.0704 (5)	
O3′	0.5229 (3)	0.56376 (5)	0.34945 (12)	0.0766 (6)	
O4′	0.8266 (3)	0.46389 (5)	0.49620 (11)	0.0721 (6)	
O4C	0.2932 (4)	0.20905 (6)	−0.01637 (14)	0.0909 (7)	

N1C	0.4294 (3)	0.33992 (6)	0.01710 (12)	0.0571 (5)	
N2C	0.5611 (4)	0.37320 (7)	0.11443 (14)	0.0772 (7)	
N3C	0.6713 (4)	0.34779 (7)	−0.06396 (14)	0.0668 (6)	
C1C	0.4139 (5)	0.35240 (8)	0.08614 (16)	0.0697 (8)	
C2C	0.6752 (5)	0.37470 (8)	0.06255 (18)	0.0705 (8)	
H2C	0.785 (5)	0.3879 (9)	0.0685 (17)	0.074 (9)*	
C3C	0.5974 (4)	0.35420 (7)	0.00232 (15)	0.0578 (6)	
C4C	0.2524 (9)	0.34396 (14)	0.1246 (3)	0.1032 (14)	
H4CA	0.207 (7)	0.3175 (15)	0.123 (3)	0.154 (19)*	
H4CB	0.284 (7)	0.3513 (15)	0.170 (3)	0.15 (2)*	
H4CC	0.140 (10)	0.3572 (18)	0.104 (3)	0.19 (3)*	
C5C	0.2834 (4)	0.31870 (8)	−0.03207 (18)	0.0639 (7)	
H5CA	0.260 (4)	0.3289 (8)	−0.0824 (17)	0.069 (8)*	
H5CB	0.161 (5)	0.3213 (8)	−0.0124 (16)	0.075 (9)*	
C6C	0.3292 (5)	0.27923 (8)	−0.03625 (16)	0.0651 (7)	
H6CA	0.454 (5)	0.2757 (9)	−0.0532 (18)	0.085 (10)*	
H6CB	0.231 (4)	0.2679 (8)	−0.0697 (16)	0.063 (8)*	
C7C	0.3174 (4)	0.22757 (8)	0.03984 (18)	0.0659 (7)	
C14C	0.332 (6)	0.2182 (8)	0.1204 (10)	0.068 (6)	0.5318
C15C	0.390 (4)	0.2413 (5)	0.1819 (15)	0.068 (3)	0.5318
H15C	0.419867	0.265318	0.173166	0.082*	0.5318
C16C	0.403 (2)	0.2292 (5)	0.2561 (9)	0.093 (4)	0.5318
H16C	0.434781	0.245824	0.295117	0.112*	0.5318
C17C	0.370 (2)	0.1927 (6)	0.2740 (8)	0.112 (5)	0.5318
H17C	0.385648	0.184515	0.323553	0.135*	0.5318
C18C	0.310 (2)	0.1691 (4)	0.2119 (7)	0.101 (6)	0.5318
H18C	0.277796	0.145168	0.220181	0.121*	0.5318
C19C	0.300 (3)	0.1817 (6)	0.1385 (13)	0.088 (4)	0.5318
H19C	0.270497	0.165123	0.099208	0.105*	0.5318
C8C	0.322 (6)	0.2090 (9)	0.1134 (10)	0.062 (6)	0.4682
C13C	0.364 (4)	0.2293 (6)	0.176 (2)	0.081 (6)	0.4682
H13C	0.392618	0.253879	0.173808	0.097*	0.4682
C12C	0.362 (3)	0.2123 (5)	0.2448 (12)	0.099 (6)	0.4682
H12C	0.390847	0.225357	0.289514	0.119*	0.4682
C11C	0.317 (3)	0.1770 (6)	0.2460 (7)	0.094 (5)	0.4682
H11C	0.317949	0.165177	0.291564	0.113*	0.4682
C10C	0.269 (3)	0.1580 (6)	0.1779 (9)	0.109 (6)	0.4682
H10C	0.238908	0.133490	0.179162	0.130*	0.4682
C9C	0.266 (4)	0.1735 (6)	0.1132 (13)	0.081 (5)	0.4682
H9C	0.226439	0.160916	0.068431	0.097*	0.4682
O1A	0.8622 (4)	0.60568 (6)	0.72428 (15)	0.1031 (8)	
O2A	0.9845 (4)	0.57753 (6)	0.82685 (13)	0.0913 (7)	
O4A	0.7325 (4)	0.47827 (10)	0.98395 (13)	0.1178 (10)	
N2A	0.8422 (3)	0.50522 (6)	0.62493 (12)	0.0589 (5)	
N3A	0.9160 (4)	0.57788 (7)	0.75940 (15)	0.0722 (7)	
C1A	0.9167 (4)	0.48799 (7)	0.68826 (14)	0.0548 (6)	
C2A	0.8300 (4)	0.54068 (8)	0.64394 (16)	0.0613 (7)	
H2A	0.782 (4)	0.5591 (8)	0.6103 (18)	0.076 (9)*	

C3A	0.8979 (4)	0.54472 (7)	0.71862 (15)	0.0574 (6)
C4A	0.9548 (6)	0.44854 (9)	0.6922 (2)	0.0726 (8)
H4AA	1.089 (6)	0.4430 (11)	0.708 (2)	0.112 (14)*
H4AB	0.892 (5)	0.4370 (10)	0.731 (2)	0.106 (12)*
H4AC	0.902 (6)	0.4365 (11)	0.648 (3)	0.122 (14)*
C5A	1.0501 (4)	0.50018 (10)	0.82398 (15)	0.0628 (7)
H5AA	1.146 (4)	0.5180 (8)	0.8411 (16)	0.073 (9)*
H5AB	1.104 (5)	0.4746 (10)	0.8180 (18)	0.085 (10)*
C6A	0.9251 (5)	0.49971 (10)	0.88285 (16)	0.0666 (7)
H6AA	1.011 (4)	0.4945 (8)	0.9322 (18)	0.078 (9)*
H6AB	0.859 (5)	0.5241 (10)	0.8861 (18)	0.091 (11)*
C7A	0.6892 (4)	0.46458 (9)	0.92272 (16)	0.0726 (8)
C8A	0.5226 (4)	0.44060 (9)	0.90204 (17)	0.0701 (8)
C9A	0.4877 (5)	0.42069 (9)	0.8363 (2)	0.0777 (9)
H9A	0.580 (4)	0.4208 (8)	0.8021 (17)	0.072 (9)*
C10A	0.3229 (6)	0.39958 (10)	0.8191 (3)	0.0967 (13)
H10A	0.307 (6)	0.3863 (11)	0.770 (2)	0.117 (14)*
C11A	0.1962 (6)	0.39897 (12)	0.8675 (3)	0.1073 (15)
H11A	0.073 (7)	0.3852 (12)	0.856 (3)	0.135 (16)*
C12A	0.2295 (6)	0.41829 (12)	0.9333 (3)	0.1003 (13)
H12A	0.134 (6)	0.4175 (11)	0.969 (2)	0.115 (13)*
C13A	0.3934 (5)	0.43885 (11)	0.9514 (2)	0.0867 (10)
H13A	0.422 (6)	0.4556 (11)	0.993 (2)	0.107 (14)*
O1B	0.2377 (4)	0.64048 (6)	0.62852 (13)	0.0840 (6)
O2B	0.4848 (4)	0.67270 (7)	0.67579 (13)	0.0956 (8)
O4B	0.6319 (4)	0.77703 (6)	0.50557 (12)	0.0850 (7)
N1B	0.6714 (3)	0.64843 (6)	0.56085 (12)	0.0595 (5)
N2B	0.5676 (4)	0.60475 (6)	0.47891 (13)	0.0670 (6)
N3B	0.4023 (4)	0.65101 (7)	0.62963 (14)	0.0713 (7)
C1B	0.7086 (4)	0.62802 (7)	0.50247 (16)	0.0645 (7)
C2B	0.4352 (5)	0.61020 (8)	0.52319 (17)	0.0656 (7)
H2B	0.320 (4)	0.5970 (8)	0.5189 (16)	0.066 (8)*
C3B	0.4962 (4)	0.63698 (7)	0.57283 (15)	0.0596 (7)
C4B	0.8810 (5)	0.63092 (11)	0.4683 (2)	0.0961 (11)
H4BA	0.890475	0.655102	0.449353	0.144*
H4BB	0.873150	0.613816	0.427700	0.144*
H4BC	0.991440	0.625719	0.505677	0.144*
C5B	0.7922 (5)	0.67798 (8)	0.5974 (2)	0.0694 (8)
H5BA	0.807 (5)	0.6749 (9)	0.652 (2)	0.087 (10)*
H5BB	0.912 (5)	0.6750 (8)	0.5815 (16)	0.072 (9)*
C6B	0.7111 (5)	0.71471 (8)	0.57400 (17)	0.0683 (8)
H6BA	0.786 (4)	0.7336 (8)	0.6008 (16)	0.063 (8)*
H6BB	0.574 (5)	0.7165 (8)	0.5825 (17)	0.078 (9)*
C7B	0.6616 (4)	0.75204 (8)	0.46585 (16)	0.0633 (7)
C8B	0.6546 (4)	0.75459 (8)	0.38362 (16)	0.0656 (7)
C9B	0.6406 (5)	0.72461 (11)	0.3370 (2)	0.0789 (9)
H9B	0.642 (4)	0.7020 (8)	0.3596 (16)	0.065 (9)*
C10B	0.6313 (6)	0.72971 (15)	0.2597 (2)	0.0979 (12)

H10B	0.631 (5)	0.7072 (11)	0.233 (2)	0.111 (13)*
C11B	0.6431 (6)	0.76410 (15)	0.2314 (2)	0.1012 (12)
H11B	0.643 (6)	0.7687 (12)	0.175 (3)	0.139 (16)*
C12B	0.6565 (6)	0.79407 (14)	0.2768 (2)	0.0951 (11)
H12B	0.670 (7)	0.8222 (16)	0.256 (3)	0.17 (2)*
C13B	0.6609 (5)	0.78897 (11)	0.3529 (2)	0.0802 (9)
H13B	0.664 (5)	0.8100 (9)	0.3852 (19)	0.082 (10)*
O1′	0.6210 (4)	0.41366 (6)	0.24229 (12)	0.0924 (8)
H1′	0.593 (6)	0.4002 (12)	0.194 (3)	0.130 (15)*
O2′	0.4848 (4)	0.45805 (6)	0.17062 (11)	0.0929 (8)
H3′	0.540 (5)	0.5769 (11)	0.397 (2)	0.111 (13)*
H4′	0.829 (6)	0.4799 (11)	0.538 (2)	0.118 (13)*
C1′	0.6075 (3)	0.47064 (6)	0.29968 (12)	0.0478 (5)
C2′	0.5473 (4)	0.50641 (7)	0.29381 (14)	0.0538 (6)
H2′	0.485 (4)	0.5175 (8)	0.2465 (16)	0.066 (8)*
C3′	0.5826 (4)	0.52839 (7)	0.35727 (14)	0.0547 (6)
C4′	0.6741 (4)	0.51454 (7)	0.42558 (14)	0.0547 (6)
H4′A	0.695 (4)	0.5297 (8)	0.4690 (16)	0.066 (8)*
C5′	0.7340 (4)	0.47867 (7)	0.43047 (13)	0.0538 (6)
C6′	0.7015 (4)	0.45642 (7)	0.36715 (14)	0.0525 (6)
H6′	0.745 (4)	0.4308 (7)	0.3716 (14)	0.056 (7)*
C7′	0.5633 (4)	0.44730 (7)	0.23118 (14)	0.0547 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1C	0.0824 (16)	0.1000 (17)	0.1057 (18)	−0.0177 (14)	0.0339 (14)	0.0013 (13)
O2C	0.0938 (16)	0.1079 (17)	0.0617 (12)	−0.0126 (14)	0.0174 (12)	−0.0190 (12)
O3C	0.0881 (14)	0.0579 (11)	0.0581 (11)	−0.0031 (10)	0.0070 (10)	−0.0047 (8)
O3A	0.0616 (11)	0.0758 (12)	0.0500 (10)	−0.0110 (9)	0.0026 (8)	0.0045 (8)
N1A	0.0514 (12)	0.0630 (12)	0.0460 (11)	−0.0034 (10)	0.0046 (9)	0.0001 (9)
O3B	0.0864 (14)	0.0615 (11)	0.0644 (12)	−0.0020 (10)	0.0164 (10)	−0.0104 (9)
O3′	0.1090 (17)	0.0550 (11)	0.0595 (12)	0.0166 (11)	−0.0012 (11)	−0.0068 (9)
O4′	0.0980 (16)	0.0601 (11)	0.0497 (11)	0.0065 (10)	−0.0089 (10)	−0.0005 (9)
O4C	0.116 (2)	0.0611 (12)	0.0930 (16)	−0.0062 (12)	0.0128 (14)	−0.0160 (11)
N1C	0.0628 (14)	0.0536 (12)	0.0546 (12)	0.0006 (10)	0.0095 (10)	−0.0075 (9)
N2C	0.104 (2)	0.0613 (14)	0.0633 (15)	0.0020 (14)	0.0076 (15)	−0.0174 (11)
N3C	0.0673 (16)	0.0680 (14)	0.0659 (15)	−0.0002 (12)	0.0147 (12)	0.0021 (12)
C1C	0.090 (2)	0.0590 (16)	0.0627 (17)	0.0081 (16)	0.0208 (16)	−0.0108 (13)
C2C	0.080 (2)	0.0572 (16)	0.0690 (19)	−0.0039 (16)	0.0005 (16)	−0.0073 (13)
C3C	0.0616 (16)	0.0537 (14)	0.0570 (15)	−0.0024 (12)	0.0075 (12)	−0.0062 (11)
C4C	0.121 (4)	0.102 (3)	0.103 (3)	0.003 (3)	0.062 (3)	−0.019 (3)
C5C	0.0621 (18)	0.0632 (16)	0.0633 (17)	−0.0010 (14)	0.0028 (14)	−0.0020 (13)
C6C	0.077 (2)	0.0599 (16)	0.0555 (16)	−0.0066 (15)	0.0039 (15)	−0.0061 (12)
C7C	0.0581 (17)	0.0605 (16)	0.0777 (19)	0.0021 (13)	0.0089 (14)	0.0006 (14)
C14C	0.056 (6)	0.054 (13)	0.098 (10)	0.007 (8)	0.024 (7)	0.010 (8)
C15C	0.065 (7)	0.081 (9)	0.059 (5)	−0.005 (7)	0.013 (5)	0.002 (7)
C16C	0.074 (6)	0.136 (13)	0.072 (8)	−0.007 (7)	0.021 (5)	0.011 (7)

C17C	0.083 (8)	0.183 (16)	0.073 (10)	0.020 (8)	0.019 (7)	0.038 (9)
C18C	0.126 (9)	0.123 (15)	0.063 (13)	0.014 (9)	0.043 (12)	0.038 (11)
C19C	0.084 (7)	0.068 (10)	0.114 (14)	0.003 (6)	0.027 (8)	0.007 (8)
C8C	0.066 (8)	0.054 (15)	0.067 (6)	0.011 (10)	0.017 (5)	0.005 (6)
C13C	0.070 (9)	0.087 (13)	0.086 (10)	−0.007 (9)	0.015 (8)	0.011 (13)
C12C	0.094 (12)	0.14 (2)	0.063 (8)	0.015 (11)	0.010 (7)	−0.002 (10)
C11C	0.093 (9)	0.155 (15)	0.036 (10)	0.032 (8)	0.021 (8)	0.029 (10)
C10C	0.150 (14)	0.101 (10)	0.088 (13)	0.036 (9)	0.056 (11)	0.020 (8)
C9C	0.100 (12)	0.058 (9)	0.095 (11)	0.005 (7)	0.044 (10)	0.007 (6)
O1A	0.137 (2)	0.0657 (14)	0.1079 (19)	0.0135 (14)	0.0244 (17)	−0.0030 (13)
O2A	0.1095 (19)	0.0871 (15)	0.0741 (15)	−0.0183 (13)	0.0079 (13)	−0.0214 (11)
O4A	0.1005 (19)	0.196 (3)	0.0587 (14)	−0.052 (2)	0.0189 (13)	−0.0193 (16)
N2A	0.0597 (13)	0.0659 (13)	0.0497 (12)	−0.0009 (11)	0.0058 (10)	0.0008 (10)
N3A	0.0755 (17)	0.0693 (16)	0.0738 (17)	−0.0062 (13)	0.0188 (14)	−0.0087 (13)
C1A	0.0532 (15)	0.0615 (15)	0.0478 (13)	−0.0055 (12)	0.0042 (11)	−0.0006 (11)
C2A	0.0597 (17)	0.0686 (17)	0.0553 (15)	0.0032 (14)	0.0094 (13)	0.0067 (13)
C3A	0.0550 (15)	0.0584 (15)	0.0587 (15)	−0.0015 (12)	0.0102 (12)	−0.0027 (12)
C4A	0.083 (2)	0.0656 (18)	0.0656 (19)	−0.0013 (17)	0.0029 (18)	−0.0013 (15)
C5A	0.0545 (16)	0.082 (2)	0.0474 (14)	−0.0103 (16)	−0.0024 (12)	0.0011 (13)
C6A	0.0629 (18)	0.084 (2)	0.0497 (15)	−0.0158 (16)	0.0029 (13)	−0.0046 (13)
C7A	0.0642 (18)	0.099 (2)	0.0526 (16)	−0.0075 (16)	0.0065 (14)	0.0075 (15)
C8A	0.0601 (17)	0.0775 (19)	0.0684 (18)	−0.0014 (15)	0.0002 (14)	0.0213 (15)
C9A	0.075 (2)	0.0714 (19)	0.080 (2)	−0.0069 (17)	−0.0042 (18)	0.0225 (16)
C10A	0.096 (3)	0.073 (2)	0.106 (3)	−0.017 (2)	−0.022 (2)	0.025 (2)
C11A	0.075 (3)	0.091 (3)	0.147 (4)	−0.015 (2)	−0.004 (3)	0.054 (3)
C12A	0.070 (2)	0.098 (3)	0.132 (4)	0.000 (2)	0.016 (3)	0.048 (3)
C13A	0.072 (2)	0.089 (2)	0.100 (3)	0.0007 (19)	0.018 (2)	0.030 (2)
O1B	0.0854 (16)	0.0831 (14)	0.0907 (16)	0.0068 (12)	0.0346 (13)	0.0075 (11)
O2B	0.119 (2)	0.0971 (17)	0.0754 (14)	−0.0060 (15)	0.0307 (14)	−0.0279 (13)
O4B	0.1183 (19)	0.0642 (12)	0.0757 (13)	0.0054 (12)	0.0259 (13)	−0.0099 (10)
N1B	0.0624 (14)	0.0547 (12)	0.0617 (13)	0.0001 (10)	0.0124 (11)	−0.0074 (10)
N2B	0.0788 (16)	0.0565 (13)	0.0677 (14)	0.0021 (12)	0.0185 (12)	−0.0091 (11)
N3B	0.0839 (19)	0.0675 (15)	0.0669 (15)	0.0051 (14)	0.0255 (13)	0.0013 (12)
C1B	0.0701 (18)	0.0575 (15)	0.0682 (17)	0.0022 (14)	0.0184 (14)	−0.0096 (13)
C2B	0.073 (2)	0.0566 (15)	0.0691 (18)	0.0000 (15)	0.0184 (15)	−0.0025 (13)
C3B	0.0700 (18)	0.0549 (14)	0.0556 (15)	0.0033 (13)	0.0160 (13)	−0.0023 (11)
C4B	0.082 (2)	0.108 (3)	0.107 (3)	−0.003 (2)	0.040 (2)	−0.027 (2)
C5B	0.071 (2)	0.0659 (17)	0.068 (2)	−0.0021 (15)	0.0047 (16)	−0.0121 (14)
C6B	0.082 (2)	0.0601 (16)	0.0617 (17)	−0.0084 (16)	0.0107 (15)	−0.0123 (13)
C7B	0.0599 (17)	0.0608 (16)	0.0692 (17)	−0.0066 (13)	0.0118 (14)	−0.0101 (13)
C8B	0.0540 (16)	0.0779 (19)	0.0640 (17)	−0.0071 (14)	0.0081 (13)	−0.0126 (14)
C9B	0.070 (2)	0.087 (2)	0.079 (2)	−0.0118 (18)	0.0120 (16)	−0.0207 (18)
C10B	0.083 (3)	0.130 (4)	0.079 (2)	−0.007 (2)	0.0084 (19)	−0.038 (3)
C11B	0.085 (3)	0.147 (4)	0.071 (2)	0.002 (3)	0.011 (2)	0.002 (3)
C12B	0.092 (3)	0.120 (3)	0.073 (2)	0.000 (2)	0.0145 (19)	0.010 (2)
C13B	0.079 (2)	0.085 (2)	0.076 (2)	−0.0051 (18)	0.0126 (17)	−0.0013 (18)
O1′	0.151 (2)	0.0591 (12)	0.0587 (12)	0.0135 (13)	−0.0021 (13)	−0.0159 (10)
O2′	0.130 (2)	0.0837 (15)	0.0529 (12)	0.0226 (14)	−0.0171 (12)	−0.0174 (10)

C1′	0.0488 (13)	0.0526 (13)	0.0419 (12)	−0.0064 (11)	0.0078 (10)	−0.0060 (10)
C2′	0.0589 (16)	0.0548 (14)	0.0457 (13)	−0.0004 (12)	0.0038 (11)	−0.0022 (11)
C3′	0.0602 (16)	0.0490 (13)	0.0540 (14)	0.0010 (12)	0.0083 (12)	−0.0047 (11)
C4′	0.0638 (16)	0.0545 (14)	0.0430 (13)	−0.0027 (12)	0.0020 (12)	−0.0084 (11)
C5′	0.0581 (15)	0.0565 (14)	0.0441 (13)	−0.0025 (12)	0.0023 (11)	−0.0014 (10)
C6′	0.0576 (15)	0.0489 (14)	0.0498 (13)	−0.0013 (12)	0.0067 (11)	−0.0038 (10)
C7′	0.0569 (15)	0.0583 (15)	0.0486 (14)	−0.0037 (12)	0.0084 (12)	−0.0073 (11)

Geometric parameters (Å, º)

O1C—N3C	1.232 (3)	C4A—H4AA	0.97 (4)
O2C—N3C	1.221 (3)	C4A—H4AB	1.00 (4)
O3C—C6C	1.440 (3)	C4A—H4AC	0.94 (5)
O3C—C7C	1.336 (3)	C5A—H5AA	0.96 (3)
O3A—C6A	1.450 (3)	C5A—H5AB	1.03 (3)
O3A—C7A	1.342 (3)	C5A—C6A	1.508 (4)
N1A—C1A	1.358 (3)	C6A—H6AA	1.00 (3)
N1A—C3A	1.380 (3)	C6A—H6AB	1.02 (4)
N1A—C5A	1.474 (3)	C7A—C8A	1.475 (4)
O3B—C6B	1.447 (3)	C8A—C9A	1.379 (5)
O3B—C7B	1.344 (3)	C8A—C13A	1.396 (5)
O3′—H3′	0.97 (4)	C9A—H9A	0.98 (3)
O3′—C3′	1.369 (3)	C9A—C10A	1.398 (5)
O4′—H4′	0.96 (4)	C10A—H10A	0.99 (4)
O4′—C5′	1.363 (3)	C10A—C11A	1.368 (7)
O4C—C7C	1.209 (4)	C11A—H11A	1.00 (5)
N1C—C1C	1.352 (3)	C11A—C12A	1.368 (7)
N1C—C3C	1.381 (3)	C12A—H12A	1.03 (4)
N1C—C5C	1.466 (3)	C12A—C13A	1.382 (6)
N2C—C1C	1.326 (4)	C13A—H13A	0.96 (4)
N2C—C2C	1.350 (4)	O1B—N3B	1.235 (3)
N3C—C3C	1.413 (3)	O2B—N3B	1.225 (3)
C1C—C4C	1.484 (5)	O4B—C7B	1.208 (3)
C2C—H2C	0.92 (3)	N1B—C1B	1.359 (3)
C2C—C3C	1.357 (4)	N1B—C3B	1.375 (3)
C4C—H4CA	1.02 (5)	N1B—C5B	1.468 (4)
C4C—H4CB	0.85 (6)	N2B—C1B	1.332 (4)
C4C—H4CC	0.95 (7)	N2B—C2B	1.360 (4)
C5C—H5CA	0.97 (3)	N3B—C3B	1.421 (3)
C5C—H5CB	1.01 (3)	C1B—C4B	1.479 (4)
C5C—C6C	1.493 (4)	C2B—H2B	0.95 (3)
C6C—H6CA	1.00 (3)	C2B—C3B	1.350 (4)
C6C—H6CB	0.94 (3)	C4B—H4BA	0.9600
C7C—C14C	1.480 (13)	C4B—H4BB	0.9600
C7C—C8C	1.489 (12)	C4B—H4BC	0.9600
C14C—C15C	1.40 (3)	C5B—H5BA	0.98 (3)
C14C—C19C	1.41 (3)	C5B—H5BB	0.96 (3)
C15C—H15C	0.9300	C5B—C6B	1.500 (4)

C15C—C16C	1.40 (3)	C6B—H6BA	0.95 (3)
C16C—H16C	0.9300	C6B—H6BB	1.02 (3)
C16C—C17C	1.41 (3)	C7B—C8B	1.480 (4)
C17C—H17C	0.9300	C8B—C9B	1.380 (4)
C17C—C18C	1.42 (2)	C8B—C13B	1.386 (5)
C18C—H18C	0.9300	C9B—H9B	0.93 (3)
C18C—C19C	1.39 (3)	C9B—C10B	1.399 (5)
C19C—H19C	0.9300	C10B—H10B	0.96 (4)
C8C—C13C	1.35 (4)	C10B—C11B	1.372 (6)
C8C—C9C	1.37 (4)	C11B—H11B	1.04 (5)
C13C—H13C	0.9300	C11B—C12B	1.367 (6)
C13C—C12C	1.39 (4)	C12B—H12B	1.11 (6)
C12C—H12C	0.9300	C12B—C13B	1.381 (5)
C12C—C11C	1.34 (3)	C13B—H13B	0.97 (3)
C11C—H11C	0.9300	O1′—H1′	0.99 (5)
C11C—C10C	1.402 (19)	O1′—C7′	1.308 (3)
C10C—H10C	0.9300	O2′—C7′	1.202 (3)
C10C—C9C	1.29 (4)	C1′—C2′	1.383 (3)
C9C—H9C	0.9300	C1′—C6′	1.383 (3)
O1A—N3A	1.228 (3)	C1′—C7′	1.492 (3)
O2A—N3A	1.228 (3)	C2′—H2′	0.98 (3)
O4A—C7A	1.203 (4)	C2′—C3′	1.388 (3)
N2A—C1A	1.331 (3)	C3′—C4′	1.384 (3)
N2A—C2A	1.356 (4)	C4′—H4′A	0.95 (3)
N3A—C3A	1.419 (4)	C4′—C5′	1.385 (4)
C1A—C4A	1.476 (4)	C5′—C6′	1.391 (3)
C2A—H2A	0.93 (3)	C6′—H6′	0.99 (3)
C2A—C3A	1.356 (4)		

C7C—O3C—C6C	116.0 (2)	C6A—C5A—H5AA	105.1 (18)
C7A—O3A—C6A	113.8 (2)	C6A—C5A—H5AB	110.2 (18)
C1A—N1A—C3A	104.7 (2)	O3A—C6A—C5A	110.0 (2)
C1A—N1A—C5A	124.2 (2)	O3A—C6A—H6AA	108.9 (17)
C3A—N1A—C5A	130.8 (2)	O3A—C6A—H6AB	110 (2)
C7B—O3B—C6B	115.5 (2)	C5A—C6A—H6AA	106.5 (18)
C3′—O3′—H3′	113 (2)	C5A—C6A—H6AB	111.7 (19)
C5′—O4′—H4′	112 (2)	H6AA—C6A—H6AB	109 (3)
C1C—N1C—C3C	105.6 (2)	O3A—C7A—C8A	114.4 (3)
C1C—N1C—C5C	124.8 (3)	O4A—C7A—O3A	122.6 (3)
C3C—N1C—C5C	129.3 (2)	O4A—C7A—C8A	123.0 (3)
C1C—N2C—C2C	107.1 (2)	C9A—C8A—C7A	123.2 (3)
O1C—N3C—C3C	116.7 (3)	C9A—C8A—C13A	119.2 (3)
O2C—N3C—O1C	123.8 (3)	C13A—C8A—C7A	117.6 (3)
O2C—N3C—C3C	119.5 (2)	C8A—C9A—H9A	120.2 (19)
N1C—C1C—C4C	124.1 (3)	C8A—C9A—C10A	119.9 (4)
N2C—C1C—N1C	111.1 (3)	C10A—C9A—H9A	119.9 (19)
N2C—C1C—C4C	124.8 (3)	C9A—C10A—H10A	115 (3)
N2C—C2C—H2C	124 (2)	C11A—C10A—C9A	119.8 (5)

N2C—C2C—C3C	108.8 (3)	C11A—C10A—H10A	125 (3)
C3C—C2C—H2C	128 (2)	C10A—C11A—H11A	122 (3)
N1C—C3C—N3C	124.9 (2)	C10A—C11A—C12A	121.0 (4)
C2C—C3C—N1C	107.5 (3)	C12A—C11A—H11A	117 (3)
C2C—C3C—N3C	127.6 (3)	C11A—C12A—H12A	120 (2)
C1C—C4C—H4CA	117 (3)	C11A—C12A—C13A	119.7 (5)
C1C—C4C—H4CB	107 (4)	C13A—C12A—H12A	120 (2)
C1C—C4C—H4CC	113 (4)	C8A—C13A—H13A	113 (3)
H4CA—C4C—H4CB	110 (5)	C12A—C13A—C8A	120.3 (5)
H4CA—C4C—H4CC	104 (5)	C12A—C13A—H13A	126 (3)
H4CB—C4C—H4CC	105 (5)	C1B—N1B—C3B	105.3 (2)
N1C—C5C—H5CA	110.2 (17)	C1B—N1B—C5B	125.1 (3)
N1C—C5C—H5CB	107.7 (17)	C3B—N1B—C5B	129.4 (2)
N1C—C5C—C6C	114.2 (3)	C1B—N2B—C2B	106.5 (2)
H5CA—C5C—H5CB	106 (2)	O1B—N3B—C3B	116.6 (3)
C6C—C5C—H5CA	109.3 (17)	O2B—N3B—O1B	123.7 (3)
C6C—C5C—H5CB	108.8 (17)	O2B—N3B—C3B	119.7 (3)
O3C—C6C—C5C	108.4 (2)	N1B—C1B—C4B	125.4 (3)
O3C—C6C—H6CA	109.5 (19)	N2B—C1B—N1B	111.1 (2)
O3C—C6C—H6CB	108.9 (17)	N2B—C1B—C4B	123.6 (3)
C5C—C6C—H6CA	110.9 (19)	N2B—C2B—H2B	124.3 (17)
C5C—C6C—H6CB	108.6 (17)	C3B—C2B—N2B	108.8 (3)
H6CA—C6C—H6CB	110 (2)	C3B—C2B—H2B	126.8 (17)
O3C—C7C—C14C	105.9 (12)	N1B—C3B—N3B	124.4 (2)
O3C—C7C—C8C	120.0 (13)	C2B—C3B—N1B	108.2 (2)
O4C—C7C—O3C	122.2 (3)	C2B—C3B—N3B	127.3 (3)
O4C—C7C—C14C	131.9 (12)	C1B—C4B—H4BA	109.5
O4C—C7C—C8C	117.9 (13)	C1B—C4B—H4BB	109.5
C15C—C14C—C7C	127 (2)	C1B—C4B—H4BC	109.5
C15C—C14C—C19C	115.6 (14)	H4BA—C4B—H4BB	109.5
C19C—C14C—C7C	118 (2)	H4BA—C4B—H4BC	109.5
C14C—C15C—H15C	119.2	H4BB—C4B—H4BC	109.5
C14C—C15C—C16C	121.7 (15)	N1B—C5B—H5BA	108 (2)
C16C—C15C—H15C	119.2	N1B—C5B—H5BB	105.4 (18)
C15C—C16C—H16C	118.7	N1B—C5B—C6B	112.0 (3)
C17C—C16C—C15C	122.5 (13)	H5BA—C5B—H5BB	111 (3)
C17C—C16C—H16C	118.7	C6B—C5B—H5BA	111 (2)
C16C—C17C—H17C	122.0	C6B—C5B—H5BB	109.9 (18)
C16C—C17C—C18C	115.9 (14)	O3B—C6B—C5B	108.0 (2)
C18C—C17C—H17C	122.0	O3B—C6B—H6BA	110.0 (17)
C17C—C18C—H18C	119.8	O3B—C6B—H6BB	107.2 (18)
C19C—C18C—C17C	120.4 (15)	C5B—C6B—H6BA	111.2 (17)
C19C—C18C—H18C	119.8	C5B—C6B—H6BB	110.5 (17)
C14C—C19C—H19C	118.2	H6BA—C6B—H6BB	110 (2)
C18C—C19C—C14C	123.6 (15)	O3B—C7B—C8B	113.5 (2)
C18C—C19C—H19C	118.2	O4B—C7B—O3B	121.7 (3)
C13C—C8C—C7C	118 (3)	O4B—C7B—C8B	124.7 (3)
C9C—C8C—C7C	119 (2)	C9B—C8B—C7B	123.1 (3)

C9C—C8C—C13C	123.6 (17)	C9B—C8B—C13B	119.3 (3)
C8C—C13C—H13C	121.2	C13B—C8B—C7B	117.6 (3)
C12C—C13C—C8C	117.7 (19)	C8B—C9B—H9B	117.2 (19)
C12C—C13C—H13C	121.2	C8B—C9B—C10B	119.1 (4)
C13C—C12C—H12C	120.3	C10B—C9B—H9B	123.6 (19)
C11C—C12C—C13C	119.5 (17)	C9B—C10B—H10B	112 (2)
C11C—C12C—H12C	120.3	C11B—C10B—C9B	120.0 (4)
C12C—C11C—H11C	120.3	C11B—C10B—H10B	127 (2)
C12C—C11C—C10C	119 (2)	C10B—C11B—H11B	122 (3)
C10C—C11C—H11C	120.3	C12B—C11B—C10B	121.5 (4)
C11C—C10C—H10C	118.8	C12B—C11B—H11B	117 (3)
C9C—C10C—C11C	122 (2)	C11B—C12B—H12B	124 (3)
C9C—C10C—H10C	118.8	C11B—C12B—C13B	118.2 (4)
C8C—C9C—H9C	121.3	C13B—C12B—H12B	118 (3)
C10C—C9C—C8C	117.4 (16)	C8B—C13B—H13B	119 (2)
C10C—C9C—H9C	121.3	C12B—C13B—C8B	121.8 (4)
C1A—N2A—C2A	105.9 (2)	C12B—C13B—H13B	119 (2)
O1A—N3A—C3A	117.2 (3)	C7′—O1′—H1′	109 (2)
O2A—N3A—O1A	123.5 (3)	C2′—C1′—C6′	121.5 (2)
O2A—N3A—C3A	119.2 (3)	C2′—C1′—C7′	117.9 (2)
N1A—C1A—C4A	124.5 (2)	C6′—C1′—C7′	120.6 (2)
N2A—C1A—N1A	112.1 (2)	C1′—C2′—H2′	123.3 (16)
N2A—C1A—C4A	123.5 (2)	C1′—C2′—C3′	118.9 (2)
N2A—C2A—H2A	124.5 (19)	C3′—C2′—H2′	117.7 (16)
N2A—C2A—C3A	109.2 (3)	O3′—C3′—C2′	117.5 (2)
C3A—C2A—H2A	126.3 (19)	O3′—C3′—C4′	122.0 (2)
N1A—C3A—N3A	125.6 (2)	C4′—C3′—C2′	120.5 (2)
C2A—C3A—N1A	108.0 (2)	C3′—C4′—H4′A	119.7 (17)
C2A—C3A—N3A	126.4 (3)	C3′—C4′—C5′	119.9 (2)
C1A—C4A—H4AA	113 (2)	C5′—C4′—H4′A	120.4 (17)
C1A—C4A—H4AB	110 (2)	O4′—C5′—C4′	122.1 (2)
C1A—C4A—H4AC	112 (3)	O4′—C5′—C6′	117.6 (2)
H4AA—C4A—H4AB	104 (3)	C4′—C5′—C6′	120.3 (2)
H4AA—C4A—H4AC	112 (3)	C1′—C6′—C5′	118.9 (2)
H4AB—C4A—H4AC	104 (3)	C1′—C6′—H6′	121.7 (15)
N1A—C5A—H5AA	107.6 (18)	C5′—C6′—H6′	119.3 (15)
N1A—C5A—H5AB	105.7 (18)	O1′—C7′—C1′	113.8 (2)
N1A—C5A—C6A	115.0 (3)	O2′—C7′—O1′	122.2 (2)
H5AA—C5A—H5AB	114 (3)	O2′—C7′—C1′	124.0 (2)