

Hydrogen-bonded co-crystal structure of benzoic acid and zwitterionic L-proline

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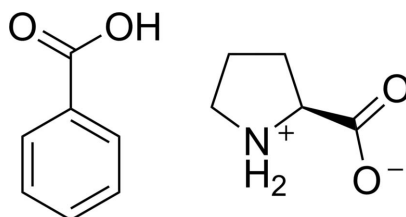
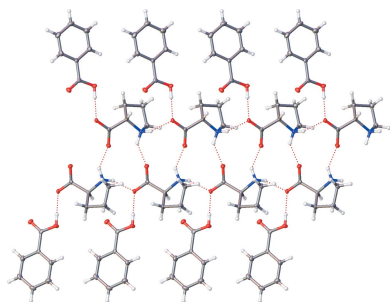
‡ Both authors contributed equally to this report.

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The title compound [systematic name: benzoic acid–pyrrolidin-1-ium-2-carboxylate (1/1)], $C_7H_6O_2 \cdot C_5H_9NO_2$, is an example of the application of non-centrosymmetric co-crystallization for the growth of a crystal containing a typically centrosymmetric component in a chiral space group. It co-crystallizes in the space group $P2_12_12_1$ and contains benzoic acid and L-proline in equal proportions. The crystal structure exhibits chains of L-proline zwitterions capped by benzoic acid molecules which form a $C(5)[R_3^3(11)]$ hydrogen-bonded network along [100]. The crystal structure is examined and compared to that of a similar co-crystal containing L-proline zwitterions and 4-aminobenzoic acid.

1. Chemical context

Non-centrosymmetric materials are of particular importance in the field of materials chemistry for the large number of symmetry-dependent properties they can possess, including circular dichroism, pyroelectricity, and non-linear optical behavior (Halasyamani & Poeppelmeier, 1998; McMillen *et al.*, 2012; Aitken *et al.*, 2009). While purposefully engineering these materials can be difficult, one method for eliminating centrosymmetry in crystalline materials is co-crystallization with an enantiopure chiral compound (Kwon *et al.*, 2006). In this way, provided that the chiral compound is not capable of racemization, the potential point groups are limited only to those which are chiral, and therefore non-centrosymmetric. The amino acid proline plays an important role in determining the structure of proteins, due to its structural rigidity. Proline has also been shown to be a good candidate for synthesizing non-centrosymmetric co-crystals. In fact, Timofeeva *et al.* (2003) reported success co-crystallizing dicyanovinyl aromatic compounds with L-proline while the same compounds would grow neat crystals when co-crystallization with L-tartaric acid was attempted.



2. Structural commentary

L-proline zwitterion (**LP**) and benzoic acid (**BA**) co-crystallize in the chiral space group $P2_12_12_1$ with one molecule of

Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots O2^i$	0.91	1.92	2.751 (3)	151
$N1-H1B\cdots O1$	0.91	2.18	2.679 (3)	114
$N1-H1B\cdots O1^{iii}$	0.91	2.08	2.782 (2)	133
$C4-H4\cdots O3^{iii}$	1.00	2.30	3.192 (3)	147
$O4-H4A\cdots O2^{iv}$	0.84	1.76	2.595 (2)	173

Symmetry codes: (i) $x - 1, y, z$; (ii) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (iii) $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$; (iv) $-x + \frac{3}{2}, -y + 1, z + \frac{1}{2}$.

L-proline and one molecule of benzoic acid in the asymmetric unit, shown in Fig. 1. The L-proline exists in its zwitterionic form within the lattice while the carboxylic acid group of the benzoic acid molecules remain protonated. Although the Flack parameter could not be used to unambiguously assign the absolute configuration, the enantiomer was reliably assigned by reference to an unchanging chiral centre in the synthetic procedure.

3. Supramolecular features

In this structure, each LP hydrogen bonds with four other LP molecules and one BA. The LP hydrogen bonding forms 1D chains along [100] via (carboxylate) $O\cdots H-N$ (pyrrolium) interactions in a $C(5)[R_3^3(11)]$ motif (Table 1). The BA molecules act as capping groups and hydrogen bond to each of the LP carboxylates through $O-H\cdots O$ (carboxylate) interactions. The complete BA-LP chains, as shown in Fig. 2, propagate along [100] and are approximately contained in (021) and (0 $\bar{2}$ 1). These chains are held together by edge-face-type $\pi-\pi$ stacking between adjacent BA molecules approximately along [010], with a ring-centroid to ring-centroid distance of 4.8451 (16) Å.

4. Database survey

Recently, the co-crystal structure of LP and *para*-amino-benzoic acid (PABA) was reported (Athimoolam & Natarajan, 2007). While the structure of BA-LP retains some

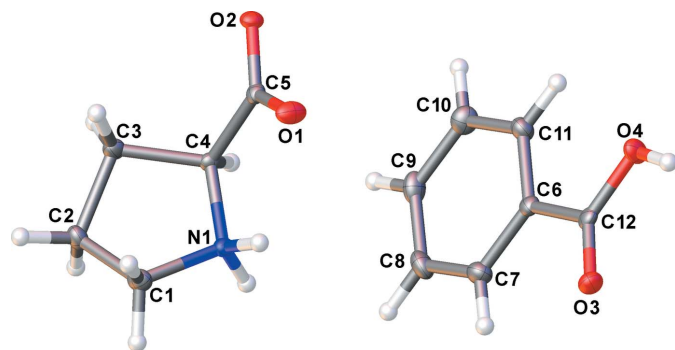


Figure 1
The asymmetric unit of the title compound, showing the atom-naming scheme. Displacement ellipsoids are shown at the 50% probability level.

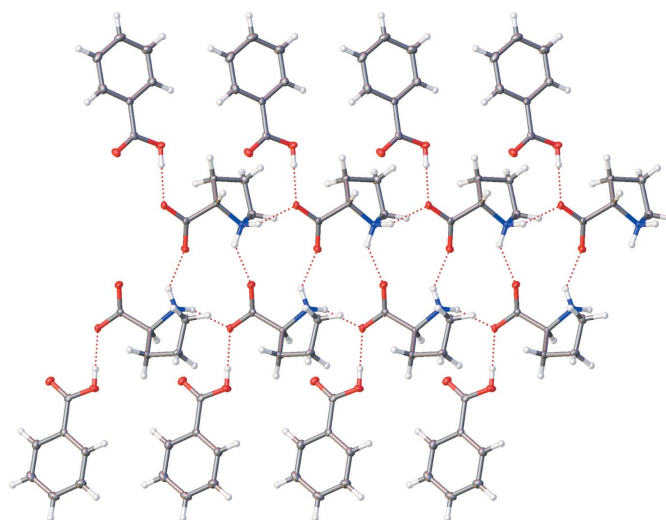


Figure 2
Diagram illustrating the hydrogen-bonding interactions in BA-LP co-crystal.

structural similarities with the PABA-LP co-crystal, due to the absence of one hydrogen-bonding moiety, the amino group, the structure of BA-LP (Fig. 3) also exhibits some important differences when compared to that of PABA-LP. The head-to-tail LP chains in PABA-LP are similar to those in BA-LP, though instead of two chains hydrogen-bonded together to form rings, the chains hydrogen bond to form a continuous 2D sheet of LP molecules. Much like BA-LP, the PABA molecules hydrogen bond to the periphery of the LP chains; however, this crystal incorporated water into the lattice and it is to these water molecules that the PABA molecules are bound. The major difference between the two structures is the presence of the hydrogen-bond donating group at the 4-position of the PABA molecules. This moiety allows the PABA molecules to bridge the LP chains in PABA-LP, a supramolecular feature absent in the title compound. The result of the lack of *para*-substitution and water in the lattice is that BA-LP forms a hydrogen-bonding network which extends in only one dimension, instead of the three-dimensional network of PABA-LP.

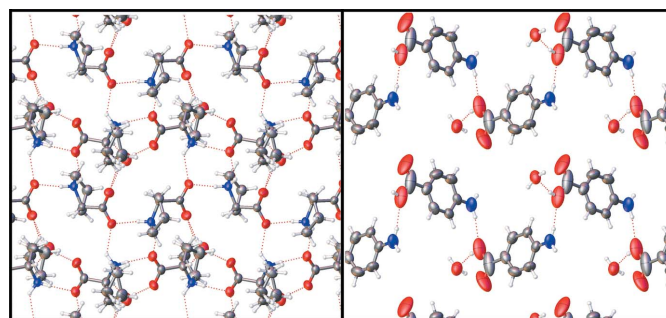


Figure 3
Diagram illustrating the hydrogen bonding network of LP in the previously reported PABA-LP co-crystal (left) and view of the PABA hydrogen-bonding network in the previously reported co-crystal (right).

5. Synthesis and crystallization

Solid **BA** (10.1 mg, 9.01×10^{-2} mmol) and **LP** (9.3 mg, 8.08×10^{-2} mmol) were added to a 25 ml scintillation vial. To this was added approximately 8 ml of ethanol followed by sonication until all solutes were fully dissolved. The loosely capped vial was then placed on an open shelf. After three weeks, colorless needle-shaped crystals of the title compound suitable for single-crystal X-ray diffraction measurements were obtained.

6. Refinement

The crystal, data collection, and refinement details are listed in Table 2. The positions of the carboxylate and pyrolium hydrogen atoms were determined from the Fourier difference map, and all other hydrogen atoms were placed in idealized positions with C–H bond lengths set to 0.93 and 0.97 Å for aryl and alkyl hydrogen atoms, respectively. These hydrogen atoms were refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ for the carboxylic acid proton on the BA molecules and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ in all other cases. No other constraints were applied to the refinement model.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_5\text{H}_9\text{NO}_2 \cdot \text{C}_7\text{H}_6\text{O}_2$
M_r	237.25
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	90
a, b, c (Å)	5.6993 (7), 12.0762 (13), 16.6839 (19)
V (Å ³)	1148.3 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.10
Crystal size (mm)	$0.1 \times 0.01 \times 0.01$
Data collection	
Diffractometer	Bruker SMART APEXII area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2013)
$T_{\text{min}}, T_{\text{max}}$	0.619, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13711, 2880, 2375
R_{int}	0.069
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.670
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.043, 0.086, 1.06
No. of reflections	2880
No. of parameters	155
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.20, -0.18
Absolute structure	Flack x determined using 824 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.5 (8)

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *olex2.solve* (Bourhis *et al.*, 2015); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Benzoic acid–pyrrolidin-1-ium-2-carboxylate (1/1)

Crystal data

$C_5H_9NO_2 \cdot C_7H_6O_2$

$M_r = 237.25$

Orthorhombic, $P2_12_12_1$

$a = 5.6993$ (7) Å

$b = 12.0762$ (13) Å

$c = 16.6839$ (19) Å

$V = 1148.3$ (2) Å³

$Z = 4$

$F(000) = 504$

$D_x = 1.372$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2011 reflections

$\theta = 3.4$ – 24.7°

$\mu = 0.10$ mm⁻¹

$T = 90$ K

Needle, colourless

$0.1 \times 0.01 \times 0.01$ mm

Data collection

Bruker SMART APEXII area detector
diffractometer

Radiation source: microfocus rotating anode,
Incoatec I μ s

Mirror optics monochromator

Detector resolution: 7.9 pixels mm⁻¹

ω and φ scans

Absorption correction: multi-scan
(SADABS; Bruker, 2013)

$T_{\min} = 0.619$, $T_{\max} = 0.746$

13711 measured reflections

2880 independent reflections

2375 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.069$

$\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -7 \rightarrow 7$

$k = -15 \rightarrow 16$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.086$

$S = 1.06$

2880 reflections

155 parameters

0 restraints

Primary atom site location: iterative

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.0827P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.20$ e Å⁻³

$\Delta\rho_{\min} = -0.18$ e Å⁻³

Absolute structure: Flack x determined using
824 quotients $[(F^-)-(F)]/[(F^+)+(F)]$ (Parsons *et al.*,
2013)
Absolute structure parameter: 0.5 (8)

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. 1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups, All N(H,H) groups At 1.5 times of: All O(H) groups 2.a Ternary CH refined with riding coordinates: C4(H4) 2.b Secondary CH2 refined with riding coordinates: N1(H1A,H1B), C1(H1C,H1D), C2(H2A,H2B), C3(H3A,H3B) 2.c Aromatic/amide H refined with riding coordinates: C7(H7), C8(H8), C9(H9), C10(H10), C11(H11) 2.d Idealised tetrahedral OH refined as rotating group: O4(H4A)

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.6846 (3)	0.69609 (14)	0.45367 (10)	0.0186 (4)
O2	0.8438 (3)	0.62955 (13)	0.34146 (9)	0.0131 (4)
N1	0.2560 (3)	0.72586 (15)	0.39137 (11)	0.0118 (4)
H1A	0.1317	0.6787	0.3892	0.014*
H1B	0.3091	0.7281	0.4428	0.014*
C1	0.1825 (5)	0.8393 (2)	0.36504 (13)	0.0161 (5)
H1C	0.2726	0.8972	0.3936	0.019*
H1D	0.0129	0.8512	0.3745	0.019*
C2	0.2381 (4)	0.8397 (2)	0.27615 (13)	0.0161 (5)
H2A	0.2546	0.9162	0.2556	0.019*
H2B	0.1152	0.8008	0.2451	0.019*
C3	0.4714 (4)	0.7775 (2)	0.27268 (14)	0.0149 (5)
H3A	0.6039	0.8275	0.2854	0.018*
H3B	0.4968	0.7451	0.2189	0.018*
C4	0.4481 (4)	0.68629 (19)	0.33630 (13)	0.0110 (5)
H4	0.3995	0.6154	0.3101	0.013*
C5	0.6756 (4)	0.66858 (18)	0.38222 (14)	0.0119 (5)
O3	0.2945 (3)	0.46855 (14)	0.70526 (9)	0.0174 (4)
O4	0.6289 (3)	0.37449 (14)	0.68623 (9)	0.0173 (4)
H4A	0.6367	0.3789	0.7364	0.026*
C6	0.3977 (4)	0.41409 (19)	0.57268 (14)	0.0125 (5)
C7	0.1924 (5)	0.4564 (2)	0.54035 (14)	0.0183 (5)
H7	0.0767	0.4870	0.5749	0.022*
C8	0.1538 (5)	0.4548 (2)	0.45852 (14)	0.0201 (6)
H8	0.0124	0.4839	0.4369	0.024*
C9	0.3232 (5)	0.41022 (19)	0.40809 (14)	0.0196 (6)
H9	0.2987	0.4095	0.3518	0.024*
C10	0.5282 (5)	0.3668 (2)	0.44000 (15)	0.0200 (6)
H10	0.6438	0.3363	0.4054	0.024*
C11	0.5651 (5)	0.3678 (2)	0.52216 (14)	0.0162 (5)
H11	0.7046	0.3369	0.5439	0.019*

C12	0.4324 (4)	0.42155 (19)	0.66114 (14)	0.0132 (5)
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Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0133 (9)	0.0308 (10)	0.0117 (8)	0.0002 (8)	-0.0019 (7)	-0.0037 (7)
O2	0.0085 (9)	0.0172 (8)	0.0135 (8)	0.0008 (7)	-0.0004 (7)	-0.0001 (7)
N1	0.0101 (11)	0.0146 (9)	0.0106 (9)	-0.0001 (8)	-0.0006 (8)	0.0010 (8)
C1	0.0155 (13)	0.0137 (11)	0.0191 (12)	0.0018 (12)	0.0015 (10)	-0.0011 (9)
C2	0.0186 (14)	0.0141 (11)	0.0155 (12)	0.0045 (11)	-0.0008 (10)	0.0015 (9)
C3	0.0139 (13)	0.0181 (12)	0.0127 (12)	0.0029 (11)	0.0020 (10)	0.0016 (10)
C4	0.0108 (12)	0.0128 (11)	0.0094 (11)	0.0004 (10)	0.0011 (9)	-0.0010 (9)
C5	0.0112 (12)	0.0116 (10)	0.0129 (11)	-0.0026 (11)	-0.0005 (10)	0.0022 (9)
O3	0.0169 (10)	0.0200 (9)	0.0152 (8)	0.0022 (8)	0.0045 (7)	0.0013 (7)
O4	0.0186 (10)	0.0231 (9)	0.0101 (8)	0.0053 (8)	-0.0017 (7)	0.0015 (7)
C6	0.0116 (12)	0.0116 (11)	0.0142 (11)	-0.0024 (10)	0.0007 (9)	0.0017 (9)
C7	0.0157 (13)	0.0174 (12)	0.0216 (13)	0.0029 (11)	0.0018 (11)	0.0008 (10)
C8	0.0196 (14)	0.0169 (12)	0.0237 (13)	0.0018 (11)	-0.0068 (12)	0.0044 (11)
C9	0.0272 (15)	0.0168 (12)	0.0147 (12)	-0.0033 (12)	-0.0059 (11)	0.0017 (9)
C10	0.0241 (14)	0.0197 (13)	0.0164 (12)	-0.0006 (12)	0.0005 (11)	-0.0027 (11)
C11	0.0160 (13)	0.0153 (11)	0.0172 (12)	0.0028 (11)	-0.0010 (10)	0.0011 (10)
C12	0.0138 (13)	0.0111 (11)	0.0146 (11)	-0.0032 (10)	0.0026 (10)	0.0027 (9)

Geometric parameters (Å, °)

O1—C5	1.239 (3)	C4—C5	1.521 (3)
O2—C5	1.266 (3)	O3—C12	1.217 (3)
N1—H1A	0.9100	O4—H4A	0.8400
N1—H1B	0.9100	O4—C12	1.324 (3)
N1—C1	1.498 (3)	C6—C7	1.386 (3)
N1—C4	1.507 (3)	C6—C11	1.391 (3)
C1—H1C	0.9900	C6—C12	1.492 (3)
C1—H1D	0.9900	C7—H7	0.9500
C1—C2	1.517 (3)	C7—C8	1.383 (3)
C2—H2A	0.9900	C8—H8	0.9500
C2—H2B	0.9900	C8—C9	1.389 (4)
C2—C3	1.528 (3)	C9—H9	0.9500
C3—H3A	0.9900	C9—C10	1.386 (4)
C3—H3B	0.9900	C10—H10	0.9500
C3—C4	1.536 (3)	C10—C11	1.387 (3)
C4—H4	1.0000	C11—H11	0.9500
H1A—N1—H1B	108.4	C5—C4—C3	112.05 (19)
C1—N1—H1A	110.0	C5—C4—H4	109.6
C1—N1—H1B	110.0	O1—C5—O2	125.8 (2)
C1—N1—C4	108.32 (18)	O1—C5—C4	118.9 (2)
C4—N1—H1A	110.0	O2—C5—C4	115.28 (19)
C4—N1—H1B	110.0	C12—O4—H4A	109.5

N1—C1—H1C	111.1	C7—C6—C11	119.5 (2)
N1—C1—H1D	111.1	C7—C6—C12	118.3 (2)
N1—C1—C2	103.39 (18)	C11—C6—C12	122.2 (2)
H1C—C1—H1D	109.0	C6—C7—H7	119.6
C2—C1—H1C	111.1	C8—C7—C6	120.8 (2)
C2—C1—H1D	111.1	C8—C7—H7	119.6
C1—C2—H2A	111.3	C7—C8—H8	120.2
C1—C2—H2B	111.3	C7—C8—C9	119.6 (3)
C1—C2—C3	102.53 (19)	C9—C8—H8	120.2
H2A—C2—H2B	109.2	C8—C9—H9	120.0
C3—C2—H2A	111.3	C10—C9—C8	120.0 (2)
C3—C2—H2B	111.3	C10—C9—H9	120.0
C2—C3—H3A	110.8	C9—C10—H10	119.9
C2—C3—H3B	110.8	C9—C10—C11	120.3 (2)
C2—C3—C4	104.55 (19)	C11—C10—H10	119.9
H3A—C3—H3B	108.9	C6—C11—H11	120.1
C4—C3—H3A	110.8	C10—C11—C6	119.9 (2)
C4—C3—H3B	110.8	C10—C11—H11	120.1
N1—C4—C3	104.87 (18)	O3—C12—O4	123.7 (2)
N1—C4—H4	109.6	O3—C12—C6	122.7 (2)
N1—C4—C5	110.90 (18)	O4—C12—C6	113.5 (2)
C3—C4—H4	109.6		
N1—C1—C2—C3	-39.6 (2)	C7—C6—C11—C10	1.6 (4)
N1—C4—C5—O1	-6.0 (3)	C7—C6—C12—O3	-4.2 (3)
N1—C4—C5—O2	176.36 (18)	C7—C6—C12—O4	177.2 (2)
C1—N1—C4—C3	-4.2 (2)	C7—C8—C9—C10	0.7 (4)
C1—N1—C4—C5	117.0 (2)	C8—C9—C10—C11	-0.1 (4)
C1—C2—C3—C4	37.3 (2)	C9—C10—C11—C6	-1.0 (4)
C2—C3—C4—N1	-20.6 (2)	C11—C6—C7—C8	-1.0 (4)
C2—C3—C4—C5	-141.01 (19)	C11—C6—C12—O3	174.9 (2)
C3—C4—C5—O1	110.8 (2)	C11—C6—C12—O4	-3.7 (3)
C3—C4—C5—O2	-66.8 (3)	C12—C6—C7—C8	178.1 (2)
C4—N1—C1—C2	27.4 (2)	C12—C6—C11—C10	-177.5 (2)
C6—C7—C8—C9	-0.1 (4)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O2 ⁱ	0.91	1.92	2.751 (3)	151
N1—H1B \cdots O1	0.91	2.18	2.679 (3)	114
N1—H1B \cdots O1 ⁱⁱ	0.91	2.08	2.782 (2)	133
C4—H4 \cdots O3 ⁱⁱⁱ	1.00	2.30	3.192 (3)	147
O4—H4A \cdots O2 ^{iv}	0.84	1.76	2.595 (2)	173

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1/2, -y+3/2, -z+1$; (iii) $-x+1/2, -y+1, z-1/2$; (iv) $-x+3/2, -y+1, z+1/2$.