

2-(4-Nitrophenoxy)benzoic acid: a three-dimensional hydrogen-bonded framework in a triclinic structure having $Z' = 3$

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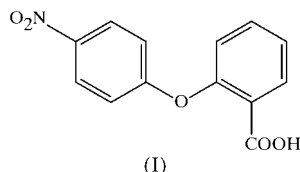
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The title compound, $C_{13}H_9NO_5$, crystallizes in space group $P\bar{1}$, with $Z' = 3$. The molecules are linked by $O-H\cdots O$ hydrogen bonds [$H\cdots O = 1.79$ – 1.81 Å, $O\cdots O = 2.625$ (3)– 2.648 (3) Å and $O-H\cdots O = 172$ – 176°] into two types of $R_2^2(8)$ dimer, only one of which is centrosymmetric. An extensive series of soft hydrogen bonds, of $C-H\cdots O$ and $C-H\cdots\pi$ (arene) types, links the dimers into a three-dimensional framework.

Comment

Persulfate oxidation of substituted 2-aryloxybenzoic acids yields asymmetrically substituted bis(salicylates), whose formation has been ascribed to the 2-4 coupling of phenoxy radicals (Thomson & Wylie, 1966). We report here the molecular and supramolecular structure of one such precursor compound, namely 2-(4-nitrophenoxy)benzoic acid, (I).



Compound (I) crystallizes in the triclinic space group $P\bar{1}$, with $Z' = 3$ (Fig. 1). In each of the three independent molecules, the two aryl rings are both rotated away from the plane of the central C/O/C fragment, as shown by the leading torsion angles (Table 1). Likewise, each of the nitro and carboxy groups is rotated away from the plane of the adjacent aryl ring. Comparison of the corresponding values for the three molecules is sufficient to rule out the possibility of any additional symmetry.

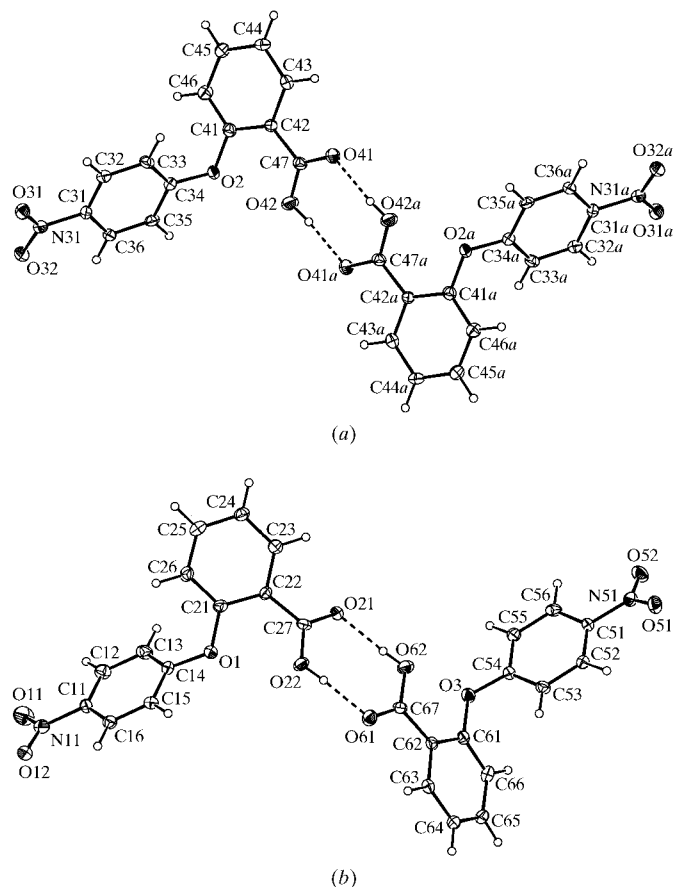


Figure 1

The independent molecules of (I), showing the atom-labelling scheme and the dimers formed by the $O-H\cdots O$ hydrogen bonding. (a) The centrosymmetric dimer formed by the type 2 molecules, where atoms labelled with the suffix *a* are at the symmetry position ($1-x$, $1-y$, $1-z$). (b) The dimer formed by the type 1 and type 3 molecules. Displacement ellipsoids are drawn at the 30% probability level.

The C–O distances within the carboxy groups are consistent with the fully ordered locations of the carboxy H atoms as deduced from difference maps. In each molecule, the central C–O–C angle has a value significantly larger than the idealized tetrahedral angle. The remaining bond lengths and angles show no unusual values.

Molecules of types 1 and 3, containing atoms O1 and O3, respectively (Fig. 1a), are linked into hydrogen-bonded dimers by two independent $O-H\cdots O$ hydrogen bonds, both of which are short for their type and nearly linear (Table 2). By contrast, molecules of type 2, containing atom O2 (Fig. 1b), are linked by pairs of $O-H\cdots O$ hydrogen bonds into centrosymmetric $R_2^2(8)$ (Bernstein *et al.*, 1995) dimers. With the centrosymmetric dimer centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, the centroid of the non-centrosymmetric dimer is at approximately (0.265, 0.225, 0.416), thus precluding the possibility of any additional inversion centres.

The two types of dimer are linked by an extensive series of soft hydrogen bonds (Braga *et al.*, 1995; Desiraju & Steiner, 1999) into a continuous three-dimensional framework of considerable complexity. However, the descriptive analysis of the framework formation is eased by the adoption of the

substructure approach (Gregson *et al.*, 2000). The dimeric units formed by the O—H···O hydrogen bonds are linked by the three strongest C—H···O hydrogen bonds (the first three such entries in Table 2, all having C—H···O angles greater than 160°) into two distinct types of chain running parallel to the [001] direction. These chains are then linked by two weaker C—H···O hydrogen bonds (the fourth and fifth such entries in Table 2, with C—H···O angles of ~140° but with H···O distances shorter than 2.50 Å). The resulting framework is further reinforced, albeit weakly, by the remaining C—H···O hydrogen bonds (which have H···O distances slightly longer than 2.50 Å) and by a single C—H···π(arene) hydrogen bond.

The centrosymmetric dimers formed by the type 2 molecules are linked by a single C—H···O hydrogen bond. Atom C46 in the molecule at (x, y, z) , which forms part of the centrosymmetric dimer centred at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, acts as a hydrogen-bond donor to nitro atom O31 in the type 2 molecule at $(1 - x, 1 - y, 2 - z)$, which forms part of the corresponding dimer centred at $(\frac{1}{2}, \frac{1}{2}, \frac{3}{2})$. Propagation of this hydrogen bond then generates a chain of rings running parallel to [001] containing $R_2^2(8)$ rings centred at $(\frac{1}{2}, \frac{1}{2}, n + \frac{1}{2})$ ($n = \text{zero or integer}$) and $R_2^2(20)$ rings centred at $(\frac{1}{2}, \frac{1}{2}, n)$ ($n = \text{zero or integer}$) (Fig. 2).

Molecules of types 1 and 3 are also linked into a [001] chain, but this is more complex than that formed by the type 2 molecules and its formation involves two C—H···O hydrogen bonds. In the first such interaction, atom C26 in the type 1 molecule at (x, y, z) acts as a hydrogen-bond donor to nitro atom O51 in the type 3 molecule at $(x, y, -1 + z)$, so linking the dimers formed by molecules 1 and 3 into a $C_2^2(18)[R_2^2(8)]$ chain of rings (Fig. 3).

In the second of these interactions, atom C13 in the type 1 molecule at (x, y, z) acts as a donor to nitro atom O52 in the type 3 molecule at $(1 - x, -y, 1 - z)$, thereby generating a centrosymmetric four-molecule aggregate centred at $(\frac{1}{2}, 0, \frac{1}{2})$ and containing two $R_2^2(8)$ rings and one $R_4^4(40)$ ring (Fig. 3). The effect of the $R_4^4(40)$ motif is to link the $C_2^2(18)[R_2^2(8)]$

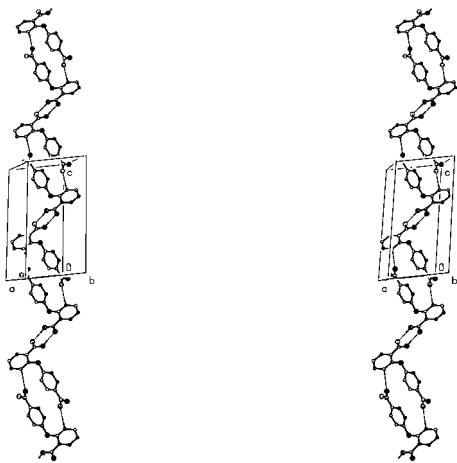


Figure 2

A stereoview of part of the crystal structure of (I), showing the formation of a [001] chain of $R_2^2(8)$ and $R_2^2(20)$ rings formed by type 2 molecules only. For clarity, H atoms not involved in the motif shown have been omitted.

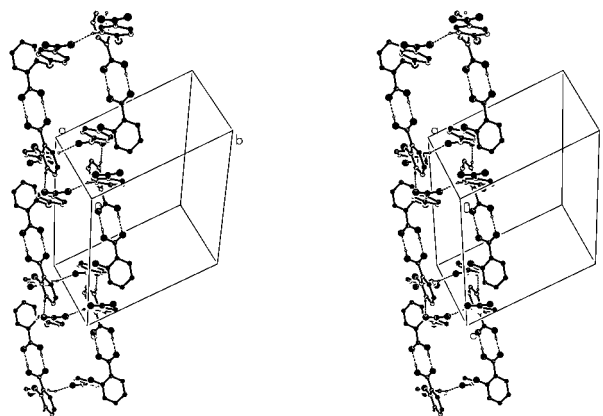


Figure 3

A stereoview of part of the crystal structure of (I), showing the formation of a complex chain along [001] containing $R_2^2(8)$, $R_4^4(20)$ and $R_4^4(40)$ rings and built from type 1 and type 3 molecules only. For clarity, H atoms not involved in the motif shown have been omitted.

chains of rings into pairs, forming a complex chain enclosing $R_4^4(20)$ rings centred at $(\frac{1}{2}, 0, n)$ ($n = \text{zero or integer}$) alternating with $R_4^4(40)$ rings centred at $(\frac{1}{2}, 0, n + \frac{1}{2})$ ($n = \text{zero or integer}$) (Fig. 3).

There are thus chains of type 2 molecules running along $(\frac{1}{2}, \frac{1}{2}, z)$, and chains containing type 1 and type 3 molecules running along $(\frac{1}{2}, 0, z)$. Two further C—H···O hydrogen bonds suffice to link these two types of chain into a single framework. Atom C16 in the type 1 molecule at (x, y, z) , which lies in the chain along $(\frac{1}{2}, 0, z)$, acts as a hydrogen-bond donor to nitro atom O32 in the type 2 molecule at $(-1 + x, y, -1 + z)$, which forms part of the chain along $(-\frac{1}{2}, \frac{1}{2}, z)$. Finally, atom C52 in the type 3 molecule at (x, y, z) acts as a donor to nitro atom O31 in the type 2 molecule at $(1 - x, 1 - y, 2 - z)$, which lies in the chain along $(\frac{1}{2}, \frac{1}{2}, z)$. Propagation of these two hydrogen bonds by translation and inversion links all of the [001] chain, and the three remaining hydrogen bonds simply reinforce the resulting framework.

The pattern of the C—H···O hydrogen bonds is itself sufficient to preclude any possible additional symmetry; for example, the nitro O atoms in the type 1 molecule, O11 and O12, do not act as hydrogen-bond acceptors, while both of the O atoms in the type 3 molecule, O51 and O52, are acceptors of C—H···O hydrogen bonds.

In addition to the hydrogen bonds, there is a short dipolar interaction involving the type 3 molecules only. The C61—O3 bonds in the molecules at (x, y, z) and $(-x, -y, 1 - z)$ are antiparallel; the corresponding O···C^{vii} and O···O^{vii} distances [symmetry code: (vii) $-x, -y, 1 - z$] are 2.978 (4) and 2.758 (3) Å, respectively, and the C—O···C^{vii} angle is 112.7 (2)°. In this respect, this interaction is reminiscent of the type II interaction between antiparallel pairs of carbonyl groups (Allen *et al.*, 1998).

Experimental

A sample of (I) was prepared by the Ullmann reaction of 2-chlorobenzoic acid with 4-nitrophenol, according to the procedure published by Thomson & Wylie (1966). Crystals suitable for single-

crystal X-ray diffraction were grown by slow evaporation of a solution in ethanol (m.p. 435–437 K).

Crystal data

$C_{13}H_9NO_5$	$Z = 6$
$M_r = 259.21$	$D_x = 1.518 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.8495 (6) \text{ \AA}$	Cell parameters from 7578 reflections
$b = 14.0847 (15) \text{ \AA}$	$\theta = 2.9\text{--}27.5^\circ$
$c = 17.2325 (18) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$\alpha = 113.187 (4)^\circ$	$T = 120 (2) \text{ K}$
$\beta = 98.515 (6)^\circ$	Lath, colourless
$\gamma = 96.400 (7)^\circ$	$0.15 \times 0.06 \times 0.02 \text{ mm}$
$V = 1701.5 (3) \text{ \AA}^3$	

Data collection

Nonius KappaCCD diffractometer	2621 reflections with $I > 2\sigma(I)$
φ scans, and ω scans with κ offsets	$R_{\text{int}} = 0.122$
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)	$\theta_{\text{max}} = 27.5^\circ$
$T_{\text{min}} = 0.966$, $T_{\text{max}} = 0.998$	$h = -9 \rightarrow 10$
14 193 measured reflections	$k = -18 \rightarrow 18$
7578 independent reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2]$
$wR(F^2) = 0.149$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.87$	$(\Delta/\sigma)_{\text{max}} = 0.001$
7578 reflections	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
517 parameters	$\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

C27–O21	1.226 (4)	C27–O22	1.314 (4)
C47–O41	1.245 (4)	C47–O42	1.297 (4)
C67–O61	1.234 (4)	C67–O62	1.297 (4)
C14–O1–C21	120.1 (3)	C54–O3–C61	118.4 (3)
C34–O2–C41	119.2 (3)		
C13–C14–O1–C21	43.0 (5)	C12–C11–N11–O11	8.5 (5)
C33–C34–O2–C41	–20.9 (5)	C32–C31–N31–O31	–11.9 (5)
C53–C54–O3–C61	–9.5 (5)	C52–C51–N51–O51	–19.2 (5)
C14–O1–C21–C22	–153.2 (3)	C21–C22–C27–O21	150.2 (4)
C34–O2–C41–C42	129.4 (3)	C41–C42–C47–O41	–169.0 (3)
C54–O3–C61–C62	115.8 (4)	C61–C62–C67–O61	170.8 (3)

Crystals of (I) are triclinic; space group $P\bar{1}$ was selected and confirmed by the subsequent structure analysis. All H atoms were located from difference maps and then treated as riding atoms, with C–H distances of 0.95 \AA and O–H distances of 0.84 \AA , and with $U_{\text{iso}}(\text{H})$ values of $1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{O})$. All H atoms were fully ordered. Examination of the refined structure using ADDSYM in PLATON (Spek, 2003) revealed no possible additional symmetry. The quality of the crystals obtained was always poor and this fact may underlie both the low proportion (35%) of the reflections labelled ‘observed’, even at $120 (2) \text{ K}$, and the fairly high merging index (0.12).

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997);

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

Cg1 is the centroid of the C61–C66 ring in the type 3 molecule; soft hydrogen bonds are listed in the order in which they are discussed in the *Comment* section.

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O22–H22 \cdots O61	0.84	1.79	2.625 (3)	175
O42–H42 \cdots O41 ⁱ	0.84	1.81	2.648 (3)	172
O62–H62 \cdots O21	0.84	1.80	2.637 (3)	176
C46–H46 \cdots O31 ⁱⁱ	0.95	2.49	3.413 (5)	163
C26–H26 \cdots O51 ⁱⁱⁱ	0.95	2.36	3.268 (5)	161
C13–H13 \cdots O52 ^{iv}	0.95	2.50	3.422 (5)	163
C16–H16 \cdots O32 ^v	0.95	2.48	3.241 (5)	138
C52–H52 \cdots O31 ⁱⁱ	0.95	2.35	3.153 (5)	142
C32–H32 \cdots O51 ⁱⁱ	0.95	2.54	3.388 (5)	149
C44–H44 \cdots O22 ^{vi}	0.95	2.53	3.370 (5)	147
C55–H55 \cdots Cg1 ^{vii}	0.95	2.87	3.745 (4)	154

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, 1-y, 2-z$; (iii) $x, y, z-1$; (iv) $1-x, -y, 1-z$; (v) $x-1, y, z-1$; (vi) $-x, 1-y, 1-z$; (vii) $-x, -y, 1-z$.

program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England; the authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants that have provided computing facilities for this work. JLW thanks CNPq and FAPERJ for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1719). Services for accessing these data are described at the back of the journal.

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2-(4-Nitrophenoxy)benzoic acid

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$C_{13}H_9NO_5$	$Z = 6$
$M_r = 259.21$	$F(000) = 804$
Triclinic, $P1$	$D_x = 1.518 \text{ Mg m}^{-3}$
Hall symbol: $-P 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.8495 (6) \text{ \AA}$	Cell parameters from 7578 reflections
$b = 14.0847 (15) \text{ \AA}$	$\theta = 2.9\text{--}27.5^\circ$
$c = 17.2325 (18) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$\alpha = 113.187 (4)^\circ$	$T = 120 \text{ K}$
$\beta = 98.515 (6)^\circ$	Lath, colourless
$\gamma = 96.400 (7)^\circ$	$0.15 \times 0.06 \times 0.02 \text{ mm}$
$V = 1701.5 (3) \text{ \AA}^3$	

Data collection

Nonius KappaCCD diffractometer	14193 measured reflections
Radiation source: rotating anode	7578 independent reflections
Graphite monochromator	2621 reflections with $I > 2\sigma(I)$
φ scans, and ω scans with κ offsets	$R_{\text{int}} = 0.122$
Absorption correction: multi-scan (<i>SORTAV</i> ; Blessing, 1995, 1997)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.9^\circ$
$T_{\text{min}} = 0.966$, $T_{\text{max}} = 0.998$	$h = -9 \rightarrow 10$
	$k = -18 \rightarrow 18$
	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.060$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.149$	H-atom parameters constrained
$S = 0.87$	
7578 reflections	
517 parameters	
0 restraints	

$$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$$

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.0187 (4)	0.1229 (3)	-0.0777 (2)	0.0279 (9)
C12	0.1217 (4)	0.0594 (3)	-0.0579 (3)	0.0351 (10)
C13	0.2194 (5)	0.0945 (3)	0.0254 (3)	0.0366 (10)
C14	0.2098 (4)	0.1926 (3)	0.0860 (2)	0.0309 (10)
C15	0.1044 (4)	0.2551 (3)	0.0661 (2)	0.0299 (10)
C16	0.0073 (4)	0.2202 (3)	-0.0169 (2)	0.0301 (10)
N11	-0.0840 (4)	0.0867 (3)	-0.1663 (2)	0.0379 (9)
O11	-0.0900 (3)	-0.0047 (3)	-0.21700 (19)	0.0578 (9)
O12	-0.1585 (3)	0.1489 (2)	-0.18541 (17)	0.0397 (7)
O1	0.2959 (3)	0.2316 (2)	0.17212 (16)	0.0397 (7)
C21	0.4668 (4)	0.2191 (3)	0.1929 (2)	0.0304 (10)
C22	0.5221 (4)	0.2166 (3)	0.2730 (2)	0.0258 (9)
C23	0.6955 (4)	0.2054 (3)	0.2947 (2)	0.0295 (9)
C24	0.8102 (5)	0.1993 (3)	0.2396 (2)	0.0326 (10)
C25	0.7506 (5)	0.2027 (3)	0.1621 (3)	0.0355 (10)
C26	0.5800 (5)	0.2123 (3)	0.1377 (2)	0.0315 (10)
C27	0.4122 (4)	0.2223 (3)	0.3364 (2)	0.0272 (9)
O21	0.4402 (3)	0.1792 (2)	0.38526 (16)	0.0336 (7)
O22	0.2868 (3)	0.2771 (2)	0.33782 (17)	0.0363 (7)
C31	0.6951 (4)	0.4867 (3)	0.9405 (2)	0.0254 (9)
C32	0.5916 (4)	0.5564 (3)	0.9325 (2)	0.0296 (10)
C33	0.4840 (4)	0.5317 (3)	0.8531 (2)	0.0299 (10)
C34	0.4823 (4)	0.4370 (3)	0.7847 (2)	0.0269 (9)
C35	0.5890 (4)	0.3693 (3)	0.7936 (2)	0.0286 (9)
C36	0.6959 (4)	0.3930 (3)	0.8722 (2)	0.0284 (9)
N31	0.8058 (4)	0.5127 (3)	1.0247 (2)	0.0301 (8)
O31	0.8254 (3)	0.6029 (2)	1.08152 (16)	0.0351 (7)
O32	0.8757 (3)	0.4430 (2)	1.03572 (16)	0.0359 (7)
O2	0.3813 (3)	0.40673 (19)	0.70293 (15)	0.0315 (7)
C41	0.2375 (4)	0.4532 (3)	0.6932 (2)	0.0290 (9)
C42	0.2178 (4)	0.4952 (3)	0.6321 (2)	0.0238 (9)
C43	0.0677 (4)	0.5371 (3)	0.6216 (2)	0.0288 (9)
C44	-0.0600 (4)	0.5360 (3)	0.6696 (2)	0.0315 (10)
C45	-0.0362 (4)	0.4928 (3)	0.7285 (2)	0.0307 (10)
C46	0.1107 (4)	0.4507 (3)	0.7408 (2)	0.0313 (10)
C47	0.3440 (4)	0.4989 (3)	0.5764 (2)	0.0281 (9)
O41	0.3275 (3)	0.5521 (2)	0.53363 (17)	0.0368 (7)
O42	0.4660 (3)	0.4433 (2)	0.57366 (18)	0.0414 (7)
C51	0.4107 (4)	0.1204 (3)	0.8066 (2)	0.0256 (9)
C52	0.2999 (4)	0.1897 (3)	0.8082 (2)	0.0277 (9)
C53	0.1912 (4)	0.1766 (3)	0.7321 (2)	0.0288 (9)

C54	0.2001 (4)	0.0936 (3)	0.6564 (2)	0.0259 (9)
C55	0.3143 (4)	0.0262 (3)	0.6548 (2)	0.0274 (9)
C56	0.4215 (4)	0.0390 (3)	0.7307 (2)	0.0296 (10)
N51	0.5205 (4)	0.1341 (3)	0.8876 (2)	0.0330 (8)
O51	0.5453 (3)	0.2213 (2)	0.94948 (17)	0.0400 (7)
O52	0.5826 (3)	0.0590 (2)	0.89088 (17)	0.0416 (7)
O3	0.0995 (3)	0.07454 (19)	0.57755 (15)	0.0313 (7)
C61	-0.0347 (4)	0.1314 (3)	0.5753 (2)	0.0262 (9)
C62	-0.0291 (4)	0.2005 (3)	0.5357 (2)	0.0251 (9)
C63	-0.1677 (4)	0.2546 (3)	0.5351 (2)	0.0275 (9)
C64	-0.3088 (4)	0.2373 (3)	0.5701 (2)	0.0309 (10)
C65	-0.3178 (4)	0.1630 (3)	0.6031 (2)	0.0302 (10)
C66	-0.1799 (4)	0.1107 (3)	0.6072 (2)	0.0304 (10)
C67	0.1095 (4)	0.2182 (3)	0.4896 (2)	0.0293 (10)
O61	0.0909 (3)	0.2709 (2)	0.44728 (16)	0.0368 (7)
O62	0.2432 (3)	0.1729 (2)	0.49515 (18)	0.0416 (7)
H12	0.1260	-0.0076	-0.1007	0.042*
H13	0.2915	0.0520	0.0405	0.044*
H15	0.0985	0.3216	0.1091	0.036*
H16	-0.0660	0.2623	-0.0319	0.036*
H23	0.7353	0.2019	0.3481	0.035*
H24	0.9281	0.1928	0.2553	0.039*
H25	0.8287	0.1983	0.1241	0.043*
H26	0.5411	0.2141	0.0835	0.038*
H22	0.2276	0.2731	0.3736	0.054*
H32	0.5939	0.6204	0.9805	0.035*
H33	0.4126	0.5790	0.8456	0.036*
H35	0.5891	0.3060	0.7453	0.034*
H36	0.7684	0.3461	0.8792	0.034*
H43	0.0523	0.5670	0.5809	0.035*
H44	-0.1618	0.5647	0.6618	0.038*
H45	-0.1228	0.4919	0.7615	0.037*
H46	0.1247	0.4205	0.7813	0.038*
H42	0.5271	0.4491	0.5391	0.062*
H52	0.2977	0.2463	0.8611	0.033*
H53	0.1128	0.2232	0.7320	0.035*
H55	0.3194	-0.0291	0.6017	0.033*
H56	0.5011	-0.0071	0.7307	0.035*
H63	-0.1646	0.3040	0.5102	0.033*
H64	-0.3998	0.2767	0.5713	0.037*
H65	-0.4191	0.1474	0.6232	0.036*
H66	-0.1846	0.0609	0.6317	0.036*
H62	0.3025	0.1760	0.4592	0.062*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.027 (2)	0.034 (3)	0.024 (2)	0.0047 (18)	0.0035 (17)	0.015 (2)

C12	0.035 (2)	0.031 (3)	0.038 (3)	0.0082 (19)	0.007 (2)	0.012 (2)
C13	0.034 (2)	0.039 (3)	0.046 (3)	0.0153 (19)	0.008 (2)	0.026 (2)
C14	0.030 (2)	0.044 (3)	0.026 (2)	0.0115 (19)	0.0109 (18)	0.019 (2)
C15	0.024 (2)	0.035 (3)	0.032 (2)	0.0086 (18)	0.0061 (18)	0.014 (2)
C16	0.026 (2)	0.035 (3)	0.034 (2)	0.0059 (18)	0.0082 (18)	0.020 (2)
N11	0.0277 (18)	0.047 (3)	0.035 (2)	0.0076 (18)	0.0065 (16)	0.013 (2)
O11	0.0543 (19)	0.047 (2)	0.048 (2)	0.0119 (16)	-0.0015 (16)	-0.0013 (18)
O12	0.0338 (15)	0.055 (2)	0.0375 (18)	0.0166 (14)	0.0084 (13)	0.0248 (16)
O1	0.0332 (15)	0.065 (2)	0.0297 (17)	0.0244 (14)	0.0098 (13)	0.0234 (16)
C21	0.028 (2)	0.036 (3)	0.034 (2)	0.0157 (18)	0.0116 (18)	0.018 (2)
C22	0.029 (2)	0.029 (2)	0.024 (2)	0.0105 (17)	0.0108 (17)	0.0114 (19)
C23	0.032 (2)	0.026 (2)	0.029 (2)	0.0077 (17)	0.0058 (18)	0.009 (2)
C24	0.025 (2)	0.035 (3)	0.033 (3)	0.0029 (17)	0.0090 (19)	0.010 (2)
C25	0.034 (2)	0.036 (3)	0.041 (3)	0.0095 (19)	0.019 (2)	0.015 (2)
C26	0.037 (2)	0.035 (3)	0.032 (2)	0.0132 (19)	0.0132 (19)	0.020 (2)
C27	0.020 (2)	0.027 (2)	0.029 (2)	0.0077 (17)	0.0001 (17)	0.006 (2)
O21	0.0299 (14)	0.0499 (19)	0.0305 (16)	0.0148 (13)	0.0079 (12)	0.0240 (15)
O22	0.0351 (15)	0.0465 (19)	0.0409 (18)	0.0196 (14)	0.0208 (13)	0.0247 (15)
C31	0.028 (2)	0.028 (2)	0.021 (2)	0.0054 (18)	0.0054 (17)	0.011 (2)
C32	0.026 (2)	0.031 (3)	0.032 (2)	0.0061 (18)	0.0091 (18)	0.012 (2)
C33	0.026 (2)	0.031 (3)	0.037 (3)	0.0109 (18)	0.0071 (19)	0.018 (2)
C34	0.026 (2)	0.034 (3)	0.025 (2)	0.0077 (18)	0.0081 (17)	0.015 (2)
C35	0.028 (2)	0.030 (3)	0.031 (2)	0.0125 (18)	0.0136 (18)	0.011 (2)
C36	0.025 (2)	0.036 (3)	0.030 (2)	0.0113 (18)	0.0075 (18)	0.018 (2)
N31	0.0268 (18)	0.036 (2)	0.032 (2)	0.0098 (17)	0.0099 (16)	0.016 (2)
O31	0.0399 (15)	0.0310 (18)	0.0284 (17)	0.0079 (13)	0.0042 (13)	0.0069 (15)
O32	0.0369 (15)	0.0381 (18)	0.0375 (17)	0.0142 (14)	0.0071 (13)	0.0193 (15)
O2	0.0351 (15)	0.0396 (18)	0.0232 (16)	0.0174 (13)	0.0047 (12)	0.0143 (14)
C41	0.029 (2)	0.029 (2)	0.025 (2)	0.0061 (18)	0.0026 (17)	0.008 (2)
C42	0.026 (2)	0.023 (2)	0.024 (2)	0.0084 (16)	0.0060 (16)	0.0097 (19)
C43	0.029 (2)	0.029 (2)	0.027 (2)	0.0033 (18)	0.0014 (17)	0.012 (2)
C44	0.025 (2)	0.034 (3)	0.038 (2)	0.0118 (18)	0.0114 (18)	0.013 (2)
C45	0.032 (2)	0.029 (3)	0.031 (2)	0.0040 (18)	0.0087 (18)	0.012 (2)
C46	0.037 (2)	0.026 (2)	0.033 (2)	0.0088 (18)	0.0110 (19)	0.013 (2)
C47	0.024 (2)	0.027 (3)	0.026 (2)	0.0069 (18)	0.0019 (17)	0.005 (2)
O41	0.0388 (16)	0.0472 (19)	0.0393 (17)	0.0161 (13)	0.0129 (13)	0.0297 (16)
O42	0.0404 (17)	0.053 (2)	0.051 (2)	0.0219 (15)	0.0247 (14)	0.0336 (17)
C51	0.025 (2)	0.031 (3)	0.023 (2)	0.0069 (18)	0.0030 (17)	0.014 (2)
C52	0.028 (2)	0.031 (3)	0.024 (2)	0.0086 (18)	0.0069 (17)	0.011 (2)
C53	0.027 (2)	0.030 (3)	0.031 (2)	0.0104 (17)	0.0037 (18)	0.013 (2)
C54	0.024 (2)	0.031 (3)	0.024 (2)	0.0054 (18)	0.0044 (17)	0.013 (2)
C55	0.028 (2)	0.027 (2)	0.026 (2)	0.0072 (18)	0.0059 (17)	0.0088 (19)
C56	0.025 (2)	0.028 (3)	0.042 (3)	0.0096 (17)	0.0102 (19)	0.020 (2)
N51	0.0306 (19)	0.042 (3)	0.033 (2)	0.0079 (18)	0.0104 (16)	0.022 (2)
O51	0.0453 (17)	0.042 (2)	0.0274 (17)	0.0066 (14)	0.0032 (13)	0.0108 (16)
O52	0.0426 (16)	0.046 (2)	0.0445 (19)	0.0159 (15)	0.0032 (14)	0.0275 (17)
O3	0.0362 (15)	0.0337 (17)	0.0275 (16)	0.0147 (12)	0.0066 (12)	0.0143 (14)
C61	0.032 (2)	0.025 (2)	0.020 (2)	0.0121 (17)	0.0049 (17)	0.0061 (19)

C62	0.027 (2)	0.027 (2)	0.019 (2)	0.0080 (17)	0.0028 (16)	0.0069 (19)
C63	0.029 (2)	0.029 (2)	0.025 (2)	0.0052 (18)	0.0036 (17)	0.013 (2)
C64	0.031 (2)	0.037 (3)	0.025 (2)	0.0136 (18)	0.0070 (18)	0.010 (2)
C65	0.031 (2)	0.032 (3)	0.026 (2)	0.0090 (19)	0.0106 (18)	0.009 (2)
C66	0.042 (2)	0.025 (2)	0.026 (2)	0.0049 (18)	0.0124 (18)	0.010 (2)
C67	0.021 (2)	0.035 (3)	0.027 (2)	0.0087 (18)	0.0027 (17)	0.007 (2)
O61	0.0439 (16)	0.0413 (19)	0.0376 (18)	0.0183 (14)	0.0160 (13)	0.0240 (16)
O62	0.0346 (16)	0.058 (2)	0.048 (2)	0.0205 (15)	0.0186 (13)	0.0311 (17)

Geometric parameters (Å, °)

C11—C12	1.375 (5)	C36—H36	0.95
C11—C16	1.381 (5)	N31—O31	1.237 (4)
C11—N11	1.474 (5)	N31—O32	1.239 (4)
C12—C13	1.386 (5)	O2—C41	1.388 (4)
C12—H12	0.95	C41—C46	1.386 (5)
C13—C14	1.384 (5)	C41—C42	1.394 (5)
C13—H13	0.95	C42—C43	1.395 (5)
C14—C15	1.376 (5)	C42—C47	1.488 (5)
C14—O1	1.392 (4)	C43—C44	1.393 (4)
C15—C16	1.382 (5)	C43—H43	0.95
C15—H15	0.95	C44—C45	1.375 (5)
C16—H16	0.95	C44—H44	0.95
N11—O12	1.225 (4)	C45—C46	1.380 (5)
N11—O11	1.229 (4)	C45—H45	0.95
O1—C21	1.385 (4)	C46—H46	0.95
C21—C26	1.379 (5)	O42—H42	0.84
C21—C22	1.398 (5)	C51—C52	1.372 (5)
C22—C23	1.400 (4)	C51—C56	1.381 (5)
C22—C27	1.473 (5)	C51—N51	1.458 (4)
C23—C24	1.388 (4)	C52—C53	1.387 (5)
C23—H23	0.95	C52—H52	0.95
C24—C25	1.369 (5)	C53—C54	1.385 (5)
C24—H24	0.95	C53—H53	0.95
C25—C26	1.381 (5)	C54—C55	1.372 (5)
C25—H25	0.95	C54—O3	1.374 (4)
C26—H26	0.95	C55—C56	1.380 (5)
C27—O21	1.226 (4)	C55—H55	0.95
C47—O41	1.245 (4)	C56—H56	0.95
C67—O61	1.234 (4)	N51—O52	1.230 (4)
C27—O22	1.314 (4)	N51—O51	1.240 (4)
C47—O42	1.297 (4)	O3—C61	1.398 (4)
C67—O62	1.297 (4)	C61—C66	1.387 (4)
O22—H22	0.84	C61—C62	1.392 (5)
C31—C32	1.377 (5)	C62—C63	1.397 (5)
C31—C36	1.381 (5)	C62—C67	1.493 (5)
C31—N31	1.460 (4)	C63—C64	1.380 (4)
C32—C33	1.388 (5)	C63—H63	0.95

C32—H32	0.95	C64—C65	1.375 (5)
C33—C34	1.386 (5)	C64—H64	0.95
C33—H33	0.95	C65—C66	1.384 (5)
C34—C35	1.374 (5)	C65—H65	0.95
C34—O2	1.385 (4)	C66—H66	0.95
C35—C36	1.376 (5)	O62—H62	0.84
C35—H35	0.95		
C12—C11—C16	122.1 (4)	C46—C41—O2	118.9 (3)
C12—C11—N11	119.5 (4)	C46—C41—C42	121.4 (3)
C16—C11—N11	118.5 (4)	O2—C41—C42	119.6 (3)
C11—C12—C13	119.1 (4)	C41—C42—C43	117.8 (3)
C11—C12—H12	120.4	C41—C42—C47	125.4 (3)
C13—C12—H12	120.4	C43—C42—C47	116.8 (3)
C14—C13—C12	118.8 (4)	C44—C43—C42	121.4 (4)
C14—C13—H13	120.6	C44—C43—H43	119.3
C12—C13—H13	120.6	C42—C43—H43	119.3
C15—C14—C13	121.8 (4)	C45—C44—C43	118.9 (4)
C15—C14—O1	115.5 (4)	C45—C44—H44	120.6
C13—C14—O1	122.6 (4)	C43—C44—H44	120.6
C14—C15—C16	119.4 (4)	C44—C45—C46	121.4 (3)
C14—C15—H15	120.3	C44—C45—H45	119.3
C16—C15—H15	120.3	C46—C45—H45	119.3
C11—C16—C15	118.8 (4)	C45—C46—C41	119.1 (4)
C11—C16—H16	120.6	C45—C46—H46	120.5
C15—C16—H16	120.6	C41—C46—H46	120.5
O12—N11—O11	123.7 (4)	O41—C47—O42	122.9 (3)
O12—N11—C11	118.5 (4)	O41—C47—C42	119.9 (3)
O11—N11—C11	117.8 (4)	O42—C47—C42	117.1 (3)
C14—O1—C21	120.1 (3)	C47—O42—H42	109.5
C26—C21—O1	121.2 (3)	C52—C51—C56	121.9 (3)
C26—C21—C22	121.1 (3)	C52—C51—N51	118.7 (3)
O1—C21—C22	117.7 (3)	C56—C51—N51	119.4 (3)
C21—C22—C23	117.8 (3)	C51—C52—C53	119.6 (4)
C21—C22—C27	125.6 (3)	C51—C52—H52	120.2
C23—C22—C27	116.5 (3)	C53—C52—H52	120.2
C24—C23—C22	121.2 (4)	C54—C53—C52	118.2 (4)
C24—C23—H23	119.4	C54—C53—H53	120.9
C22—C23—H23	119.4	C52—C53—H53	120.9
C25—C24—C23	118.9 (4)	C55—C54—O3	115.3 (3)
C25—C24—H24	120.6	C55—C54—C53	121.9 (3)
C23—C24—H24	120.6	O3—C54—C53	122.8 (3)
C24—C25—C26	121.7 (4)	C54—C55—C56	119.7 (4)
C24—C25—H25	119.1	C54—C55—H55	120.1
C26—C25—H25	119.1	C56—C55—H55	120.1
C21—C26—C25	119.2 (4)	C55—C56—C51	118.5 (4)
C21—C26—H26	120.4	C55—C56—H56	120.7
C25—C26—H26	120.4	C51—C56—H56	120.7

O21—C27—O22	123.0 (3)	O52—N51—O51	123.9 (3)
O21—C27—C22	120.9 (3)	O52—N51—C51	118.5 (3)
O22—C27—C22	116.1 (4)	O51—N51—C51	117.6 (3)
C27—O22—H22	109.5	C54—O3—C61	118.4 (3)
C32—C31—C36	122.3 (4)	C66—C61—C62	120.9 (3)
C32—C31—N31	118.4 (3)	C66—C61—O3	118.2 (3)
C36—C31—N31	119.2 (3)	C62—C61—O3	120.7 (3)
C31—C32—C33	118.9 (4)	C61—C62—C63	118.0 (3)
C31—C32—H32	120.6	C61—C62—C67	125.3 (3)
C33—C32—H32	120.6	C63—C62—C67	116.6 (3)
C34—C33—C32	118.9 (4)	C64—C63—C62	121.0 (4)
C34—C33—H33	120.5	C64—C63—H63	119.5
C32—C33—H33	120.5	C62—C63—H63	119.5
C35—C34—O2	115.8 (3)	C65—C64—C63	120.0 (4)
C35—C34—C33	121.3 (4)	C65—C64—H64	120.0
O2—C34—C33	122.9 (3)	C63—C64—H64	120.0
C34—C35—C36	120.2 (4)	C64—C65—C66	120.3 (3)
C34—C35—H35	119.9	C64—C65—H65	119.9
C36—C35—H35	119.9	C66—C65—H65	119.9
C35—C36—C31	118.4 (4)	C65—C66—C61	119.6 (4)
C35—C36—H36	120.8	C65—C66—H66	120.2
C31—C36—H36	120.8	C61—C66—H66	120.2
O31—N31—O32	123.1 (3)	O61—C67—O62	123.7 (3)
O31—N31—C31	118.6 (3)	O61—C67—C62	120.1 (3)
O32—N31—C31	118.3 (3)	O62—C67—C62	116.2 (4)
C34—O2—C41	119.2 (3)	C67—O62—H62	109.5
C16—C11—C12—C13	-1.0 (6)	N31—C31—C36—C35	179.2 (3)
N11—C11—C12—C13	179.3 (3)	C36—C31—N31—O31	168.9 (3)
C11—C12—C13—C14	0.0 (5)	C32—C31—N31—O32	168.0 (3)
C12—C13—C14—C15	0.9 (5)	C36—C31—N31—O32	-11.2 (5)
C12—C13—C14—O1	176.5 (3)	C35—C34—O2—C41	162.2 (3)
C13—C14—C15—C16	-1.0 (5)	C34—O2—C41—C46	-54.7 (4)
O1—C14—C15—C16	-176.9 (3)	C46—C41—C42—C43	1.5 (5)
C12—C11—C16—C15	0.9 (5)	O2—C41—C42—C43	177.3 (3)
N11—C11—C16—C15	-179.4 (3)	C46—C41—C42—C47	-178.4 (3)
C14—C15—C16—C11	0.1 (5)	O2—C41—C42—C47	-2.5 (5)
C12—C11—N11—O12	-171.6 (3)	C41—C42—C43—C44	-0.8 (5)
C16—C11—N11—O12	8.7 (5)	C47—C42—C43—C44	179.0 (3)
C16—C11—N11—O11	-171.2 (3)	C42—C43—C44—C45	0.2 (5)
C15—C14—O1—C21	-141.2 (3)	C43—C44—C45—C46	-0.1 (5)
C14—O1—C21—C26	28.5 (5)	C44—C45—C46—C41	0.7 (5)
C13—C14—O1—C21	43.0 (5)	O2—C41—C46—C45	-177.3 (3)
C33—C34—O2—C41	-20.9 (5)	C42—C41—C46—C45	-1.4 (5)
C53—C54—O3—C61	-9.5 (5)	C43—C42—C47—O41	11.1 (5)
C14—O1—C21—C22	-153.2 (3)	C41—C42—C47—O42	12.4 (5)
C34—O2—C41—C42	129.4 (3)	C43—C42—C47—O42	-167.4 (3)
C54—O3—C61—C62	115.8 (4)	C56—C51—C52—C53	2.0 (5)

C12—C11—N11—O11	8.5 (5)	N51—C51—C52—C53	-178.4 (3)
C32—C31—N31—O31	-11.9 (5)	C51—C52—C53—C54	-0.7 (5)
C52—C51—N51—O51	-19.2 (5)	C52—C53—C54—C55	-1.0 (5)
C21—C22—C27—O21	150.2 (4)	C52—C53—C54—O3	-179.2 (3)
C41—C42—C47—O41	-169.0 (3)	O3—C54—C55—C56	179.8 (3)
C61—C62—C67—O61	170.8 (3)	C53—C54—C55—C56	1.4 (5)
C26—C21—C22—C23	-0.9 (6)	C54—C55—C56—C51	-0.1 (5)
O1—C21—C22—C23	-179.2 (3)	C52—C51—C56—C55	-1.6 (5)
C26—C21—C22—C27	-179.4 (3)	N51—C51—C56—C55	178.8 (3)
O1—C21—C22—C27	2.3 (6)	C52—C51—N51—O52	160.6 (3)
C21—C22—C23—C24	1.4 (5)	C56—C51—N51—O52	-19.8 (5)
C27—C22—C23—C24	180.0 (3)	C56—C51—N51—O51	160.4 (3)
C22—C23—C24—C25	-1.0 (6)	C55—C54—O3—C61	172.1 (3)
C23—C24—C25—C26	0.1 (6)	C54—O3—C61—C66	-69.4 (4)
O1—C21—C26—C25	178.3 (3)	C66—C61—C62—C63	5.0 (5)
C22—C21—C26—C25	0.1 (6)	O3—C61—C62—C63	179.6 (3)
C24—C25—C26—C21	0.3 (6)	C66—C61—C62—C67	-171.9 (3)
C23—C22—C27—O21	-28.3 (5)	O3—C61—C62—C67	2.7 (5)
C21—C22—C27—O22	-30.9 (5)	C61—C62—C63—C64	-2.2 (5)
C23—C22—C27—O22	150.6 (3)	C67—C62—C63—C64	174.9 (3)
C36—C31—C32—C33	0.1 (5)	C62—C63—C64—C65	-2.6 (5)
N31—C31—C32—C33	-179.0 (3)	C63—C64—C65—C66	4.7 (5)
C31—C32—C33—C34	0.9 (5)	C64—C65—C66—C61	-2.0 (5)
C32—C33—C34—C35	-2.2 (5)	C62—C61—C66—C65	-3.0 (5)
C32—C33—C34—O2	-178.9 (3)	O3—C61—C66—C65	-177.7 (3)
O2—C34—C35—C36	179.3 (3)	C63—C62—C67—O61	-6.2 (5)
C33—C34—C35—C36	2.4 (5)	C61—C62—C67—O62	-7.3 (5)
C34—C35—C36—C31	-1.3 (5)	C63—C62—C67—O62	175.7 (3)
C32—C31—C36—C35	0.1 (5)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O22—H22 \cdots O61	0.84	1.79	2.625 (3)	175
O42—H42 \cdots O41 ⁱ	0.84	1.81	2.648 (3)	172
O62—H62 \cdots O21	0.84	1.80	2.637 (3)	176
C46—H46 \cdots O31 ⁱⁱ	0.95	2.49	3.413 (5)	163
C26—H26 \cdots O51 ⁱⁱⁱ	0.95	2.36	3.268 (5)	161
C13—H13 \cdots O52 ^{iv}	0.95	2.50	3.422 (5)	163
C16—H16 \cdots O32 ^v	0.95	2.48	3.241 (5)	138
C52—H52 \cdots O31 ⁱⁱ	0.95	2.35	3.153 (5)	142
C32—H32 \cdots O51 ⁱⁱ	0.95	2.54	3.388 (5)	149
C44—H44 \cdots O22 ^{vi}	0.95	2.53	3.370 (5)	147
C55—H55 \cdots Cg1 ^{viii}	0.95	2.87	3.745 (4)	154

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