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Tetraphenylphosphonium hydrogen oxalate

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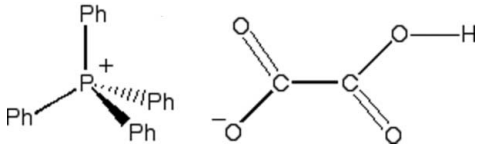
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.053; data-to-parameter ratio = 10.9.

In the title compound, $C_{24}H_{20}P^+\cdot C_2HO_4^-$, two symmetry-independent ion pairs are present. The cations aggregate into puckered sheets *via* zigzag infinite chains of sixfold phenyl embraces and parallel fourfold phenyl embraces, while the anions form hydrogen-bonded chains between the sheets of cations. In the two independent oxalate anions, the angles between the normals to the two least-squares carboxylate COO planes are unusually large, *viz*. 72.5 (1) and 82.1 (1)°.

Related literature

For a related investigation of the packing of Ph_4P^+ ions in the presence of differently shaped and/or charged anions, see: Dean *et al.* (2004). For a discussion of phenyl braces, see: Scudder & Dance (1998).

For related literature, see: Allen (2002); Braga *et al.* (2002); Chandra *et al.* (1998); Periasamy *et al.* (2004); Ramanaiah *et al.* (1999); Rodrigues *et al.* (2001).



Experimental

Crystal data

$C_{24}H_{20}P^+\cdot C_2HO_4^-$
M_r = 428.4
Triclinic, $P\overline{1}$
a = 9.517 (5) Å
b = 10.860 (7) Å
c = 22.032 (9) Å
α = 78.49 (3)°
β = 88.37 (2)°
γ = 75.13 (3)°
V = 2156 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 294 K
0.25 × 0.20 × 0.05 mm

Data collection

Nonius CAD-4 diffractometer
Absorption correction: none
8001 measured reflections
7564 independent reflections
4017 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
1 standard reflection
frequency: 30 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.053
S = 1.35
4017 reflections
367 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.91 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4C—H1O4C···O1D	1.00	1.51	2.505 (2)	180
O4D—H1O4D···O1C^{i}	1.00	1.50	2.500 (2)	180

Symmetry code: (i) $x, y-1, z$.

Data collection: *CAD-4* (Schagen *et al.*, 1989); cell refinement: *CAD-4*; data reduction: local program; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *RAELS* (Rae, 2000); molecular graphics: *ORTEPII* (Johnson, 1976) and *CrystalMaker* (CrystalMaker Software, 2005); software used to prepare material for publication: local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LN2012).

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S1. Comment

The structure of Ph_4P^+ $HC_2O_4^-$ was determined as part of a series investigating the packing of Ph_4P^+ ions in the presence of differently shaped and/or charged anions (Dean *et al.*, 2004). The structure contains recognizable Ph_4P^+ and $HC_2O_4^-$ ions, each in two crystallographically distinct forms (Figure 1). The PPh_4^+ cations, A and B, each aggregate *via* zigzag infinite chains of sixfold phenyl embraces (ZZI6PE) (Scudder & Dance, 1998) propagating parallel to the *b* axis. Within the P1A-containing chains, alternating P···P distances of 6.476 (1) and 6.609 (1) Å are found, and the P···P···P angle is 112.2 (1)°. The corresponding metrics in the chains containing P1B are 6.093 (1) and 6.684 (1) Å and 116.3 (1)°. The ZZI6PE chains are linked into puckered sheets, lying parallel to *bc*, through parallel fourfold phenyl embraces (P4PE) (Scudder & Dance, 1998) with a P1A···P1B distance of 8.072 (1) Å. The two P1A···P1A···P1B angles are 99.6 (1) and 144.3 (1)°, while the two P1B···P1B···P1A angles are 99.5 (1) and 140.9 (1)°.

Between the sheets of PPh_4^+ cations, hydrogen-bonded chains of alternating crystallographically independent $HC_2O_4^-$ anions, C and D, run parallel to the *b* axis (Figure 2). The distances between the O atoms involved in the hydrogen bonds are 2.505 (2) and 2.500 (2) Å for O4C···O1D and O4D···.O1C, respectively (Table 1). For the two independent molecules, the angle between the normals to the least squares planes defined by the two carboxylate COO groups are 72.5 (1) and 82.1 (1)°, for anions C and D, respectively. A search of the Cambridge Structural Database (CSD V5.27 2006, Allen, 2002) for structures containing uncoordinated $H_2C_2O_4$ or $HC_2O_4^-$ revealed that while there is a full spread of angles between these normals, from 0–90°, the preference is for an angle near to, or exactly, 0°. Out of 156 hits, in only 6 does this angle exceed 65° [CSD refcode AHETAI, 85.6° (Braga *et al.*, 2002); AHESUB, 69.5° (Braga *et al.*, 2002); BEYDAL, 80.3° (Periasamy, *et al.*, 2004); GUKYEQ, 70.2° (Rodrigues *et al.*, 2001); NOSXAU, 87.0° (Chandra *et al.*, 1998); XEHZEP, 75.6° (Ramanaiah *et al.*, 1999)].

S2. Experimental

Ph_4P^+ $HC_2O_4^-$ was the only crystalline product isolated from an attempt to synthesize $(Ph_4P^+)_2$ $C_2O_4^{2-}$ in crystalline form. Thus, Ph_4P^+ Br^- (0.859 g, 2.05 mmol) and $Ag_2C_2O_4$ (0.380 g, 1.25 mmol) were stirred together at ambient laboratory temperature in *ca* 15 ml of Me_2CO in a foil-wrapped vial. After 2 days, the precipitate was allowed to settle and the mother liquor was separated by decantation. Slow evaporation of the mother liquor for 6 days at ambient laboratory temperature, led to a small number of colourless plate-like crystals. The data crystal was selected from these. No further formation of *X*-ray quality crystals occurred on further evaporation of the mother liquor. The compound Ph_4P^+ $HC_2O_4^-$ is presumably a hydrolysis product of the intended $(Ph_4P^+)_2$ $C_2O_4^{2-}$.

S3. Refinement

The carbon atoms of the cations were refined anisotropcally with 12-parameter TL rigid-body thermal parameters with their centres of libration at the appropriate P atom used for each phenyl ring. The remainimg non-hydrogen atoms were

refined with single atom anisotropic thermal parameters. Hydrogen atoms were included in positions calculated each cycle (C—H = 1.00 Å), and their thermal motions were either included in the appropriate rigid group or assigned equal to U_{eq} of their bonded atom.

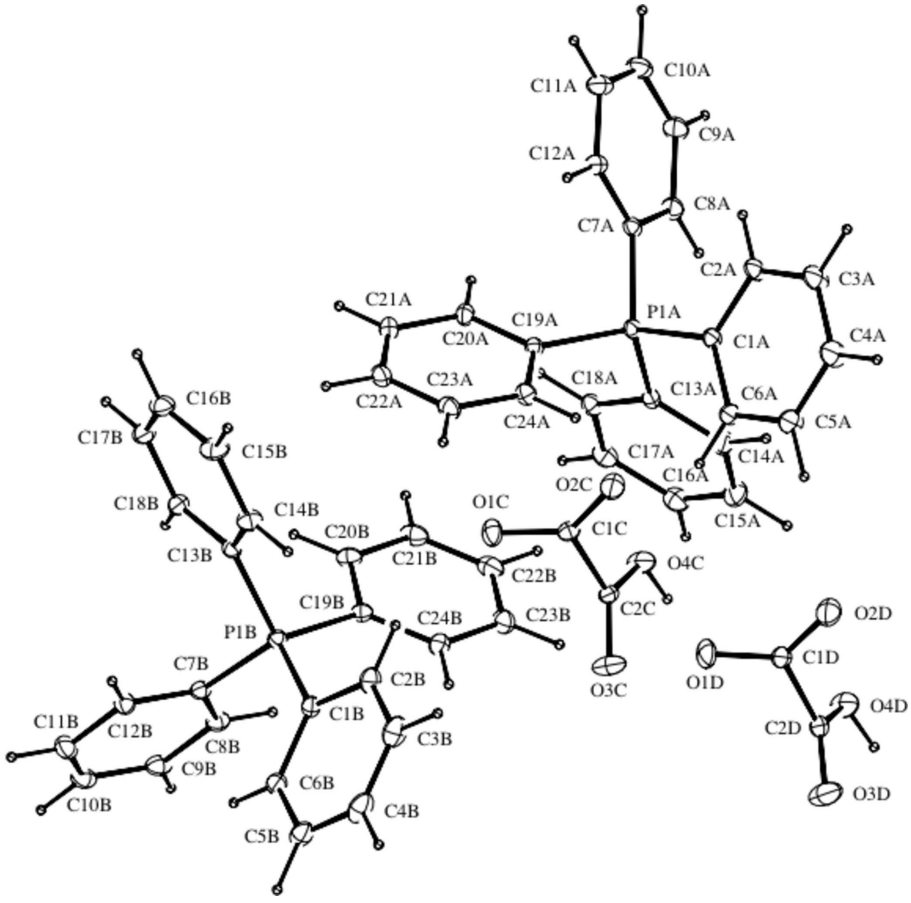

Figure 1

A view of the two independent Ph_4P^+ cations and $HC_2O_4^-$ anions, showing the labelling of the non-H atoms. Thermal ellipsoids are shown at the 50% probability levels.

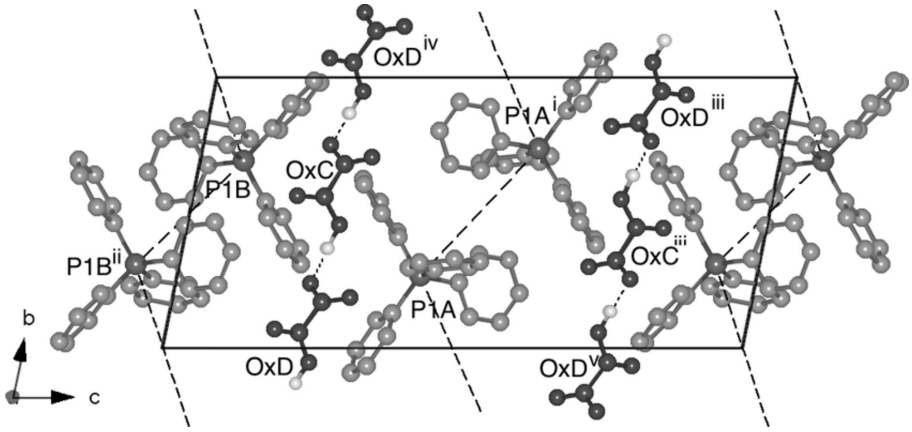

Figure 2

Projection down the *a* axis of the lattice of $Ph_4P^+HC_2O_4^-$, showing the hydrogen-bonded chains of $HC_2O_4^-$ anions (labelled OxC and OxD) propagating parallel to the *b* axis. The zigzag chains of cations are also evident. H atoms have been omitted for clarity. Symmetry operators: (i) 1 - *x*, 1 - *y*, 1 - *z*; (ii) 1 - *x*, 1 - *y*, -*z*; (iii) -*x*, 1 - *y*, 1 - *z*; (iv) *x*, 1 + *y*, *z*; v -*x*, -*y*, 1 - *z*.

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Crystal data

$C_{24}H_{20}P^+\cdot C_2HO_4^-$
M_r = 428.4
Triclinic, $P\overline{1}$
a = 9.517 (5) Å
b = 10.860 (7) Å
c = 22.032 (9) Å
α = 78.49 (3)°
β = 88.37 (2)°
γ = 75.13 (3)°
V = 2156 (2) Å^3
Z = 4
F(000) = 896.0
D_x = 1.32 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 10 reflections
θ = 10–11°
μ = 0.15 mm^{-1}
T = 294 K
Plate, colourless
0.25 × 0.20 × 0.05 mm

Data collection

Nonius CAD-4 diffractometer
ω–2*θ* scans
8001 measured reflections
7564 independent reflections
4017 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25°
h = −11→11
k = 0→12
l = −26→26
1 standard reflections every 30 min
intensity decay: none

Refinement

Refinement on *F*
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.053
S = 1.35
4017 reflections
367 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F) + 0.0004F^2]$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.91 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
P1A	0.56052 (10)	0.26506 (10)	0.42012 (5)	0.0398 (3)
C1A	0.3737 (4)	0.2877 (4)	0.4413 (2)	0.043 (1)
C2A	0.3320 (4)	0.2991 (4)	0.5014 (2)	0.056 (1)
C3A	0.1873 (4)	0.3192 (5)	0.5165 (2)	0.077 (2)
C4A	0.0856 (5)	0.3254 (5)	0.4721 (2)	0.083 (2)
C5A	0.1249 (4)	0.3135 (5)	0.4121 (2)	0.072 (1)
C6A	0.2688 (4)	0.2955 (4)	0.3967 (2)	0.052 (1)
C7A	0.6704 (4)	0.2379 (4)	0.4888 (2)	0.0432 (9)
C8A	0.7397 (4)	0.1130 (4)	0.5184 (2)	0.0572 (9)
C9A	0.8159 (5)	0.0945 (5)	0.5737 (2)	0.073 (1)
C10A	0.8248 (5)	0.2010 (5)	0.5978 (2)	0.072 (1)
C11A	0.7578 (4)	0.3250 (5)	0.5680 (2)	0.065 (1)
C12A	0.6801 (4)	0.3443 (4)	0.5135 (2)	0.0519 (8)
C13A	0.6152 (4)	0.1255 (4)	0.3853 (2)	0.043 (1)
C14A	0.5276 (5)	0.0419 (4)	0.3840 (2)	0.060 (1)
C15A	0.5776 (5)	−0.0671 (4)	0.3577 (2)	0.075 (1)
C16A	0.7157 (5)	−0.0936 (4)	0.3343 (2)	0.069 (1)
C17A	0.8027 (5)	−0.0111 (4)	0.3357 (2)	0.062 (1)
C18A	0.7541 (4)	0.0986 (4)	0.3604 (2)	0.051 (1)
C19A	0.5877 (4)	0.4074 (3)	0.3689 (2)	0.0393 (8)
C20A	0.7254 (4)	0.4290 (4)	0.3649 (2)	0.0523 (8)
C21A	0.7506 (5)	0.5365 (4)	0.3247 (2)	0.0647 (8)
C22A	0.6379 (5)	0.6222 (4)	0.2887 (2)	0.062 (1)
C23A	0.5005 (5)	0.6014 (4)	0.2915 (2)	0.060 (1)
C24A	0.4742 (4)	0.4935 (4)	0.3315 (2)	0.0495 (8)
P1B	0.55487 (11)	0.69137 (10)	0.07479 (5)	0.0416 (3)
C1B	0.3754 (4)	0.7491 (4)	0.0402 (2)	0.046 (1)
C2B	0.2553 (4)	0.7702 (4)	0.0779 (2)	0.060 (1)
C3B	0.1184 (5)	0.8189 (5)	0.0504 (3)	0.079 (1)
C4B	0.0997 (5)	0.8412 (5)	−0.0126 (3)	0.083 (2)
C5B	0.2181 (5)	0.8167 (4)	−0.0501 (2)	0.073 (2)
C6B	0.3569 (4)	0.7707 (4)	−0.0243 (2)	0.056 (1)
C7B	0.6838 (4)	0.6713 (4)	0.0148 (2)	0.045 (1)
C8B	0.7547 (4)	0.5495 (4)	0.0043 (2)	0.053 (1)
C9B	0.8469 (4)	0.5393 (5)	−0.0453 (2)	0.063 (1)
C10B	0.8675 (5)	0.6483 (5)	−0.0843 (2)	0.067 (1)
C11B	0.7974 (5)	0.7706 (5)	−0.0742 (2)	0.067 (1)
C12B	0.7071 (4)	0.7819 (4)	−0.0245 (2)	0.055 (1)
C13B	0.5938 (4)	0.8087 (3)	0.1147 (2)	0.042 (1)
C14B	0.4854 (5)	0.8997 (4)	0.1371 (2)	0.0600 (9)
C15B	0.5225 (6)	0.9842 (4)	0.1693 (2)	0.074 (1)
C16B	0.6655 (6)	0.9776 (4)	0.1793 (2)	0.068 (1)
C17B	0.7743 (5)	0.8873 (4)	0.1580 (2)	0.0630 (9)
C18B	0.7399 (4)	0.8021 (4)	0.1257 (2)	0.0518 (9)
C19B	0.5724 (4)	0.5390 (4)	0.1276 (2)	0.044 (1)

C20B	0.7021 (4)	0.4815 (4)	0.1613 (2)	0.0542 (9)
C21B	0.7158 (5)	0.3646 (4)	0.2027 (2)	0.066 (1)
C22B	0.6017 (6)	0.3070 (4)	0.2106 (2)	0.069 (1)
C23B	0.4745 (5)	0.3617 (4)	0.1773 (2)	0.069 (1)
C24B	0.4590 (4)	0.4785 (4)	0.1354 (2)	0.0557 (9)
O1C	0.1627 (3)	0.7471 (3)	0.2192 (1)	0.0695 (9)
O2C	0.0122 (4)	0.7022 (3)	0.2938 (2)	0.082 (1)
O3C	0.0257 (4)	0.5591 (3)	0.1787 (2)	0.081 (1)
O4C	0.1584 (4)	0.4521 (3)	0.2619 (1)	0.0750 (9)
C1C	0.0866 (4)	0.6785 (4)	0.2494 (2)	0.046 (1)
C2C	0.0862 (4)	0.5568 (4)	0.2260 (2)	0.043 (1)
O1D	0.1842 (4)	0.2373 (3)	0.2314 (2)	0.085 (1)
O2D	0.0341 (4)	0.1848 (3)	0.3038 (2)	0.090 (1)
O3D	0.0171 (5)	0.0683 (3)	0.1861 (2)	0.108 (1)
O4D	0.1799 (4)	−0.0537 (3)	0.2558 (1)	0.0752 (9)
C1D	0.1072 (5)	0.1684 (4)	0.2579 (2)	0.052 (1)
C2D	0.0989 (5)	0.0538 (4)	0.2292 (2)	0.053 (1)
HC2A	0.4068	0.2928	0.5336	0.059
HC3A	0.1566	0.3291	0.5594	0.096
HC4A	−0.0190	0.3389	0.4834	0.107
HC5A	0.0496	0.3178	0.3805	0.086
HC6A	0.2983	0.2881	0.3534	0.054
HC8A	0.7350	0.0369	0.5002	0.067
HC9A	0.8644	0.0045	0.5961	0.097
HC10A	0.8808	0.1872	0.6374	0.090
HC11A	0.7652	0.4011	0.5857	0.081
HC12A	0.6308	0.4345	0.4917	0.060
HC14A	0.4285	0.0599	0.4020	0.074
HC15A	0.5134	−0.1262	0.3557	0.102
HC16A	0.7525	−0.1732	0.3163	0.084
HC17A	0.9025	−0.0309	0.3185	0.077
HC18A	0.8178	0.1588	0.3606	0.061
HC20A	0.8072	0.3665	0.3913	0.065
HC21A	0.8502	0.5516	0.3220	0.088
HC22A	0.6556	0.7004	0.2601	0.075
HC23A	0.4197	0.6641	0.2647	0.078
HC24A	0.3749	0.4779	0.3334	0.062
HC2B	0.2679	0.7505	0.1240	0.066
HC3B	0.0315	0.8381	0.0769	0.102
HC4B	−0.0005	0.8755	−0.0316	0.105
HC5B	0.2034	0.8322	−0.0961	0.090
HC6B	0.4431	0.7530	−0.0512	0.061
HC8B	0.7395	0.4695	0.0322	0.060
HC9B	0.8991	0.4514	−0.0528	0.076
HC10B	0.9335	0.6393	−0.1202	0.080
HC11B	0.8121	0.8501	−0.1027	0.085
HC12B	0.6577	0.8700	−0.0165	0.063
HC14B	0.3808	0.9041	0.1299	0.077

HC15B	0.4446	1.0502	0.1853	0.104
HC16B	0.6915	1.0394	0.2024	0.083
HC17B	0.8784	0.8834	0.1659	0.082
HC18B	0.8187	0.7361	0.1102	0.065
HC20B	0.7845	0.5239	0.1556	0.064
HC21B	0.8088	0.3220	0.2270	0.085
HC22B	0.6122	0.2236	0.2413	0.083
HC23B	0.3932	0.3180	0.1831	0.089
HC24B	0.3663	0.5191	0.1107	0.066
H1O4C	0.1687	0.3663	0.2498	0.075
H1O4D	0.1730	−0.1335	0.2412	0.075

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1A	0.0307 (6)	0.0476 (7)	0.0392 (6)	−0.0103 (5)	0.0018 (5)	−0.0038 (5)
C1A	0.033 (1)	0.054 (2)	0.041 (1)	−0.010 (1)	0.0017 (9)	−0.005 (1)
C2A	0.038 (1)	0.081 (2)	0.043 (1)	−0.010 (1)	0.0065 (9)	−0.009 (2)
C3A	0.041 (1)	0.127 (3)	0.056 (1)	−0.014 (2)	0.013 (1)	−0.016 (2)
C4A	0.036 (1)	0.140 (4)	0.071 (2)	−0.020 (1)	0.011 (1)	−0.020 (2)
C5A	0.034 (1)	0.113 (3)	0.068 (2)	−0.019 (1)	0.001 (1)	−0.019 (2)
C6A	0.034 (1)	0.072 (2)	0.051 (1)	−0.013 (1)	−0.001 (1)	−0.011 (2)
C7A	0.035 (2)	0.055 (2)	0.038 (1)	−0.010 (1)	0.005 (1)	−0.006 (1)
C8A	0.052 (2)	0.060 (2)	0.053 (1)	−0.013 (1)	−0.010 (1)	0.004 (1)
C9A	0.068 (2)	0.086 (2)	0.057 (2)	−0.020 (2)	−0.019 (1)	0.010 (2)
C10A	0.059 (2)	0.109 (3)	0.047 (1)	−0.021 (2)	−0.008 (1)	−0.010 (2)
C11A	0.047 (2)	0.097 (2)	0.054 (2)	−0.013 (2)	0.000 (1)	−0.030 (2)
C12A	0.039 (1)	0.068 (1)	0.050 (1)	−0.009 (1)	0.003 (1)	−0.021 (1)
C13A	0.043 (2)	0.045 (1)	0.039 (2)	−0.012 (1)	0.004 (1)	−0.001 (1)
C14A	0.063 (2)	0.057 (1)	0.067 (2)	−0.027 (1)	0.013 (1)	−0.017 (1)
C15A	0.091 (2)	0.061 (2)	0.083 (2)	−0.031 (2)	0.016 (2)	−0.026 (1)
C16A	0.088 (2)	0.054 (1)	0.062 (2)	−0.009 (1)	0.006 (2)	−0.015 (2)
C17A	0.062 (2)	0.061 (2)	0.054 (2)	−0.001 (1)	0.006 (2)	−0.013 (2)
C18A	0.045 (1)	0.056 (1)	0.047 (2)	−0.008 (1)	0.007 (1)	−0.007 (1)
C19A	0.036 (1)	0.043 (1)	0.039 (1)	−0.009 (1)	0.005 (1)	−0.010 (1)
C20A	0.045 (1)	0.062 (1)	0.053 (2)	−0.023 (1)	0.005 (1)	−0.005 (1)
C21A	0.069 (2)	0.073 (2)	0.059 (2)	−0.039 (2)	0.007 (1)	−0.003 (1)
C22A	0.087 (2)	0.056 (1)	0.047 (2)	−0.031 (2)	0.007 (2)	−0.006 (1)
C23A	0.073 (2)	0.049 (1)	0.051 (2)	−0.013 (1)	−0.001 (2)	−0.001 (1)
C24A	0.047 (1)	0.047 (1)	0.048 (1)	−0.006 (1)	−0.001 (1)	−0.003 (1)
P1B	0.0391 (6)	0.0445 (7)	0.0407 (6)	−0.0095 (5)	−0.0008 (5)	−0.0084 (5)
C1B	0.042 (1)	0.043 (2)	0.050 (2)	−0.013 (1)	−0.001 (1)	−0.002 (1)
C2B	0.040 (1)	0.062 (2)	0.074 (1)	−0.012 (1)	0.007 (1)	−0.010 (2)
C3B	0.041 (1)	0.075 (2)	0.116 (3)	−0.010 (1)	−0.003 (1)	−0.010 (2)
C4B	0.055 (1)	0.067 (2)	0.120 (3)	−0.016 (1)	−0.030 (1)	0.006 (2)
C5B	0.072 (2)	0.063 (2)	0.080 (2)	−0.027 (2)	−0.033 (2)	0.012 (2)
C6B	0.061 (1)	0.054 (2)	0.051 (2)	−0.022 (1)	−0.013 (1)	0.004 (1)
C7B	0.040 (2)	0.053 (2)	0.045 (1)	−0.012 (1)	−0.002 (1)	−0.015 (1)

C8B	0.045 (1)	0.061 (1)	0.056 (1)	−0.009 (1)	0.001 (1)	−0.025 (1)
C9B	0.046 (2)	0.088 (2)	0.059 (2)	−0.009 (2)	0.002 (1)	−0.035 (2)
C10B	0.046 (2)	0.108 (3)	0.050 (2)	−0.018 (2)	0.004 (1)	−0.027 (2)
C11B	0.056 (2)	0.093 (2)	0.053 (1)	−0.023 (2)	0.008 (1)	−0.010 (2)
C12B	0.051 (1)	0.064 (1)	0.051 (1)	−0.018 (1)	0.004 (1)	−0.009 (1)
C13B	0.050 (2)	0.039 (2)	0.035 (2)	−0.011 (1)	0.002 (1)	−0.004 (1)
C14B	0.064 (1)	0.054 (2)	0.064 (2)	−0.008 (1)	0.004 (1)	−0.027 (1)
C15B	0.092 (2)	0.061 (2)	0.076 (2)	−0.013 (2)	−0.001 (2)	−0.035 (2)
C16B	0.101 (2)	0.053 (2)	0.055 (2)	−0.026 (2)	−0.012 (2)	−0.013 (2)
C17B	0.078 (1)	0.058 (2)	0.058 (2)	−0.029 (2)	−0.012 (2)	−0.008 (1)
C18B	0.055 (1)	0.052 (2)	0.051 (2)	−0.019 (1)	−0.003 (1)	−0.009 (1)
C19B	0.045 (2)	0.042 (1)	0.043 (2)	−0.006 (1)	−0.004 (1)	−0.012 (1)
C20B	0.057 (2)	0.047 (1)	0.052 (2)	−0.001 (1)	−0.015 (1)	−0.008 (1)
C21B	0.089 (2)	0.047 (1)	0.053 (2)	0.000 (1)	−0.017 (2)	−0.007 (1)
C22B	0.111 (3)	0.045 (1)	0.048 (2)	−0.014 (1)	−0.002 (2)	−0.009 (1)
C23B	0.095 (2)	0.055 (1)	0.060 (2)	−0.029 (2)	0.005 (2)	−0.009 (1)
C24B	0.061 (2)	0.052 (1)	0.057 (2)	−0.020 (1)	0.000 (1)	−0.010 (1)
O1C	0.092 (2)	0.049 (2)	0.078 (2)	−0.033 (2)	0.033 (2)	−0.023 (2)
O2C	0.097 (3)	0.088 (3)	0.088 (3)	−0.046 (2)	0.042 (2)	−0.056 (2)
O3C	0.097 (3)	0.065 (2)	0.079 (2)	−0.002 (2)	−0.040 (2)	−0.028 (2)
O4C	0.122 (3)	0.036 (2)	0.066 (2)	−0.020 (2)	−0.030 (2)	−0.004 (2)
C1C	0.044 (3)	0.044 (3)	0.050 (3)	−0.006 (2)	−0.002 (2)	−0.017 (2)
C2C	0.043 (2)	0.046 (3)	0.044 (3)	−0.014 (2)	−0.001 (2)	−0.014 (2)
O1D	0.129 (3)	0.059 (2)	0.087 (3)	−0.057 (2)	0.039 (2)	−0.024 (2)
O2D	0.106 (3)	0.093 (3)	0.096 (3)	−0.051 (2)	0.037 (2)	−0.049 (2)
O3D	0.154 (4)	0.076 (3)	0.100 (3)	−0.042 (2)	−0.059 (3)	−0.005 (2)
O4D	0.098 (2)	0.041 (2)	0.084 (2)	−0.010 (2)	−0.012 (2)	−0.015 (2)
C1D	0.065 (3)	0.043 (3)	0.049 (3)	−0.019 (2)	−0.001 (2)	−0.005 (2)
C2D	0.064 (3)	0.046 (3)	0.049 (3)	−0.023 (2)	0.000 (2)	0.000 (2)

Geometric parameters (Å, º)

P1A—C1A	1.792 (4)	C2B—C3B	1.382 (6)
P1A—C7A	1.795 (4)	C2B—HC2B	1.000
P1A—C13A	1.786 (4)	C3B—C4B	1.369 (7)
P1A—C19A	1.796 (4)	C3B—HC3B	1.000
C1A—C2A	1.391 (5)	C4B—C5B	1.380 (7)
C1A—C6A	1.397 (5)	C4B—HC4B	1.000
C2A—C3A	1.379 (5)	C5B—C6B	1.382 (5)
C2A—HC2A	1.000	C5B—HC5B	1.000
C3A—C4A	1.375 (6)	C6B—HC6B	1.000
C3A—HC3A	1.000	C7B—C8B	1.384 (5)
C4A—C5A	1.385 (6)	C7B—C12B	1.397 (5)
C4A—HC4A	1.000	C8B—C9B	1.387 (5)
C5A—C6A	1.376 (5)	C8B—HC8B	1.000
C5A—HC5A	1.000	C9B—C10B	1.371 (6)
C6A—HC6A	1.000	C9B—HC9B	1.000
C7A—C8A	1.383 (5)	C10B—C11B	1.383 (6)

C7A—C12A	1.396 (5)	C10B—HC10B	1.000
C8A—C9A	1.389 (5)	C11B—C12B	1.378 (5)
C8A—HC8A	1.000	C11B—HC11B	1.000
C9A—C10A	1.387 (6)	C12B—HC12B	1.000
C9A—HC9A	1.000	C13B—C14B	1.388 (5)
C10A—C11A	1.372 (6)	C13B—C18B	1.399 (5)
C10A—HC10A	1.000	C14B—C15B	1.383 (5)
C11A—C12A	1.380 (5)	C14B—HC14B	1.000
C11A—HC11A	1.000	C15B—C16B	1.366 (6)
C12A—HC12A	1.000	C15B—HC15B	1.000
C13A—C14A	1.386 (5)	C16B—C17B	1.374 (6)
C13A—C18A	1.399 (5)	C16B—HC16B	1.000
C14A—C15A	1.390 (5)	C17B—C18B	1.379 (5)
C14A—HC14A	1.000	C17B—HC17B	1.000
C15A—C16A	1.379 (6)	C18B—HC18B	1.000
C15A—HC15A	1.000	C19B—C20B	1.391 (5)
C16A—C17A	1.372 (6)	C19B—C24B	1.391 (5)
C16A—HC16A	1.000	C20B—C21B	1.386 (5)
C17A—C18A	1.376 (5)	C20B—HC20B	1.000
C17A—HC17A	1.000	C21B—C22B	1.377 (6)
C18A—HC18A	1.000	C21B—HC21B	1.000
C19A—C20A	1.387 (5)	C22B—C23B	1.365 (6)
C19A—C24A	1.394 (5)	C22B—HC22B	1.000
C20A—C21A	1.387 (5)	C23B—C24B	1.389 (5)
C20A—HC20A	1.000	C23B—HC23B	1.000
C21A—C22A	1.375 (6)	C24B—HC24B	1.000
C21A—HC21A	1.000	O1C—C1C	1.254 (4)
C22A—C23A	1.380 (6)	O2C—C1C	1.222 (4)
C22A—HC22A	1.000	O3C—C2C	1.198 (4)
C23A—C24A	1.393 (5)	O4C—C2C	1.290 (4)
C23A—HC23A	1.000	O4C—H1O4C	1.000
C24A—HC24A	1.000	C1C—C2C	1.513 (5)
P1B—C1B	1.796 (4)	O1D—C1D	1.233 (5)
P1B—C7B	1.784 (4)	O2D—C1D	1.226 (5)
P1B—C13B	1.800 (4)	O3D—C2D	1.205 (5)
P1B—C19B	1.795 (4)	O4D—C2D	1.262 (5)
C1B—C2B	1.392 (5)	O4D—H1O4D	1.000
C1B—C6B	1.401 (5)	C1D—C2D	1.524 (6)

C1A—P1A—C7A	108.9 (2)	P1B—C1B—C6B	120.0 (3)
C1A—P1A—C13A	109.4 (2)	C2B—C1B—C6B	120.4 (4)
C1A—P1A—C19A	110.8 (2)	C1B—C2B—C3B	118.7 (4)
C7A—P1A—C13A	108.7 (2)	C1B—C2B—HC2B	120.6
C7A—P1A—C19A	107.9 (2)	C3B—C2B—HC2B	120.6
C13A—P1A—C19A	111.1 (2)	C2B—C3B—C4B	121.0 (5)
P1A—C1A—C2A	120.8 (3)	C2B—C3B—HC3B	119.5
P1A—C1A—C6A	119.5 (3)	C4B—C3B—HC3B	119.5
C2A—C1A—C6A	119.7 (3)	C3B—C4B—C5B	120.4 (4)

C1A—C2A—C3A	120.0 (4)	C3B—C4B—HC4B	119.8
C1A—C2A—HC2A	120.0	C5B—C4B—HC4B	119.8
C3A—C2A—HC2A	120.0	C4B—C5B—C6B	120.0 (4)
C2A—C3A—C4A	119.5 (4)	C4B—C5B—HC5B	120.0
C2A—C3A—HC3A	120.2	C6B—C5B—HC5B	120.0
C4A—C3A—HC3A	120.2	C1B—C6B—C5B	119.2 (4)
C3A—C4A—C5A	121.5 (4)	C1B—C6B—HC6B	120.4
C3A—C4A—HC4A	119.3	C5B—C6B—HC6B	120.4
C5A—C4A—HC4A	119.3	P1B—C7B—C8B	121.6 (3)
C4A—C5A—C6A	119.1 (4)	P1B—C7B—C12B	118.9 (3)
C4A—C5A—HC5A	120.4	C8B—C7B—C12B	119.5 (4)
C6A—C5A—HC5A	120.4	C7B—C8B—C9B	119.4 (4)
C1A—C6A—C5A	120.2 (4)	C7B—C8B—HC8B	120.3
C1A—C6A—HC6A	119.9	C9B—C8B—HC8B	120.3
C5A—C6A—HC6A	119.9	C8B—C9B—C10B	120.8 (4)
P1A—C7A—C8A	120.6 (3)	C8B—C9B—HC9B	119.6
P1A—C7A—C12A	119.1 (3)	C10B—C9B—HC9B	119.6
C8A—C7A—C12A	120.3 (4)	C9B—C10B—C11B	120.3 (4)
C7A—C8A—C9A	119.3 (4)	C9B—C10B—HC10B	119.8
C7A—C8A—HC8A	120.3	C11B—C10B—HC10B	119.8
C9A—C8A—HC8A	120.3	C10B—C11B—C12B	119.4 (4)
C8A—C9A—C10A	119.9 (4)	C10B—C11B—HC11B	120.3
C8A—C9A—HC9A	120.1	C12B—C11B—HC11B	120.3
C10A—C9A—HC9A	120.1	C7B—C12B—C11B	120.6 (4)
C9A—C10A—C11A	120.8 (4)	C7B—C12B—HC12B	119.7
C9A—C10A—HC10A	119.6	C11B—C12B—HC12B	119.7
C11A—C10A—HC10A	119.6	P1B—C13B—C14B	122.6 (3)
C10A—C11A—C12A	119.7 (4)	P1B—C13B—C18B	117.7 (3)
C10A—C11A—HC11A	120.1	C14B—C13B—C18B	119.7 (4)
C12A—C11A—HC11A	120.1	C13B—C14B—C15B	119.8 (4)
C7A—C12A—C11A	120.0 (4)	C13B—C14B—HC14B	120.1
C7A—C12A—HC12A	120.0	C15B—C14B—HC14B	120.1
C11A—C12A—HC12A	120.0	C14B—C15B—C16B	120.0 (4)
P1A—C13A—C14A	122.6 (3)	C14B—C15B—HC15B	120.0
P1A—C13A—C18A	118.0 (3)	C16B—C15B—HC15B	120.0
C14A—C13A—C18A	119.4 (4)	C15B—C16B—C17B	121.0 (4)
C13A—C14A—C15A	120.0 (4)	C15B—C16B—HC16B	119.5
C13A—C14A—HC14A	120.0	C17B—C16B—HC16B	119.5
C15A—C14A—HC14A	120.0	C16B—C17B—C18B	120.0 (4)
C14A—C15A—C16A	119.9 (4)	C16B—C17B—HC17B	120.0
C14A—C15A—HC15A	120.0	C18B—C17B—HC17B	120.0
C16A—C15A—HC15A	120.0	C13B—C18B—C17B	119.5 (4)
C15A—C16A—C17A	120.2 (4)	C13B—C18B—HC18B	120.2
C15A—C16A—HC16A	119.9	C17B—C18B—HC18B	120.2
C17A—C16A—HC16A	119.9	P1B—C19B—C20B	118.9 (3)
C16A—C17A—C18A	120.7 (4)	P1B—C19B—C24B	121.2 (3)
C16A—C17A—HC17A	119.6	C20B—C19B—C24B	119.9 (4)
C18A—C17A—HC17A	119.6	C19B—C20B—C21B	119.2 (4)

C13A—C18A—C17A	119.8 (4)	C19B—C20B—HC20B	120.4
C13A—C18A—HC18A	120.1	C21B—C20B—HC20B	120.4
C17A—C18A—HC18A	120.1	C20B—C21B—C22B	120.1 (4)
P1A—C19A—C20A	119.1 (3)	C20B—C21B—HC21B	119.9
P1A—C19A—C24A	121.1 (3)	C22B—C21B—HC21B	119.9
C20A—C19A—C24A	119.7 (4)	C21B—C22B—C23B	121.2 (4)
C19A—C20A—C21A	120.5 (4)	C21B—C22B—HC22B	119.4
C19A—C20A—HC20A	119.8	C23B—C22B—HC22B	119.4
C21A—C20A—HC20A	119.8	C22B—C23B—C24B	119.5 (4)
C20A—C21A—C22A	119.6 (4)	C22B—C23B—HC23B	120.3
C20A—C21A—HC21A	120.2	C24B—C23B—HC23B	120.3
C22A—C21A—HC21A	120.2	C19B—C24B—C23B	120.0 (4)
C21A—C22A—C23A	120.7 (4)	C19B—C24B—HC24B	120.0
C21A—C22A—HC22A	119.7	C23B—C24B—HC24B	120.0
C23A—C22A—HC22A	119.7	C2C—O4C—H1O4C	119.3
C22A—C23A—C24A	120.2 (4)	O1C—C1C—O2C	126.6 (4)
C22A—C23A—HC23A	119.9	O1C—C1C—C2C	115.1 (4)
C24A—C23A—HC23A	119.9	O2C—C1C—C2C	118.3 (4)
C19A—C24A—C23A	119.3 (4)	O3C—C2C—O4C	124.3 (4)
C19A—C24A—HC24A	120.3	O3C—C2C—C1C	122.8 (4)
C23A—C24A—HC24A	120.3	O4C—C2C—C1C	112.9 (3)
C1B—P1B—C7B	108.7 (2)	C2D—O4D—H1O4D	117.7
C1B—P1B—C13B	110.6 (2)	O1D—C1D—O2D	126.8 (4)
C1B—P1B—C19B	110.3 (2)	O1D—C1D—C2D	116.2 (4)
C7B—P1B—C13B	107.4 (2)	O2D—C1D—C2D	117.0 (4)
C7B—P1B—C19B	109.8 (2)	O3D—C2D—O4D	124.9 (4)
C13B—P1B—C19B	110.0 (2)	O3D—C2D—C1D	120.9 (4)
P1B—C1B—C2B	119.5 (3)	O4D—C2D—C1D	114.1 (4)

C7A—P1A—C1A—C2A	8.2 (4)	C1B—P1B—C7B—C8B	−105.3 (3)
C7A—P1A—C1A—C6A	−172.6 (3)	C1B—P1B—C7B—C12B	71.0 (3)
C13A—P1A—C1A—C2A	126.8 (3)	C13B—P1B—C7B—C8B	135.0 (3)
C13A—P1A—C1A—C6A	−54.0 (4)	C13B—P1B—C7B—C12B	−48.7 (3)
C19A—P1A—C1A—C2A	−110.3 (3)	C19B—P1B—C7B—C8B	15.4 (4)
C19A—P1A—C1A—C6A	68.9 (4)	C19B—P1B—C7B—C12B	−168.3 (3)
C1A—P1A—C7A—C8A	97.2 (3)	C1B—P1B—C13B—C14B	24.5 (4)
C1A—P1A—C7A—C12A	−80.2 (3)	C1B—P1B—C13B—C18B	−158.6 (3)
C13A—P1A—C7A—C8A	−21.9 (4)	C7B—P1B—C13B—C14B	143.0 (3)
C13A—P1A—C7A—C12A	160.7 (3)	C7B—P1B—C13B—C18B	−40.1 (3)
C19A—P1A—C7A—C8A	−142.4 (3)	C19B—P1B—C13B—C14B	−97.6 (3)
C19A—P1A—C7A—C12A	40.2 (3)	C19B—P1B—C13B—C18B	79.3 (3)
C1A—P1A—C13A—C14A	−7.9 (4)	C1B—P1B—C19B—C20B	−177.1 (3)
C1A—P1A—C13A—C18A	174.2 (3)	C1B—P1B—C19B—C24B	2.8 (4)
C7A—P1A—C13A—C14A	110.9 (3)	C7B—P1B—C19B—C20B	63.1 (3)
C7A—P1A—C13A—C18A	−67.0 (3)	C7B—P1B—C19B—C24B	−117.0 (3)
C19A—P1A—C13A—C14A	−130.6 (3)	C13B—P1B—C19B—C20B	−54.8 (3)
C19A—P1A—C13A—C18A	51.5 (3)	C13B—P1B—C19B—C24B	125.1 (3)
C1A—P1A—C19A—C20A	156.9 (3)	P1B—C1B—C2B—C3B	177.8 (3)

C1A—P1A—C19A—C24A	−25.5 (4)
C7A—P1A—C19A—C20A	37.8 (4)
C7A—P1A—C19A—C24A	−144.6 (3)
C13A—P1A—C19A—C20A	−81.2 (3)
C13A—P1A—C19A—C24A	96.4 (3)
P1A—C1A—C2A—C3A	178.7 (4)
P1A—C1A—C2A—HC2A	−1.3
C6A—C1A—C2A—C3A	−0.5 (6)
C6A—C1A—C2A—HC2A	179.5
P1A—C1A—C6A—C5A	−179.7 (3)
P1A—C1A—C6A—HC6A	0.3
C2A—C1A—C6A—C5A	−0.5 (6)
C2A—C1A—C6A—HC6A	179.5
C1A—C2A—C3A—C4A	1.2 (7)
C1A—C2A—C3A—HC3A	−178.8
HC2A—C2A—C3A—C4A	−178.8
HC2A—C2A—C3A—HC3A	1.2
C2A—C3A—C4A—C5A	−0.8 (8)
C2A—C3A—C4A—HC4A	179.2
HC3A—C3A—C4A—C5A	179.2
HC3A—C3A—C4A—HC4A	−0.8
C3A—C4A—C5A—C6A	−0.3 (8)
C3A—C4A—C5A—HC5A	179.7
HC4A—C4A—C5A—C6A	179.7
HC4A—C4A—C5A—HC5A	−0.3
C4A—C5A—C6A—C1A	0.9 (7)
C4A—C5A—C6A—HC6A	−179.1
HC5A—C5A—C6A—C1A	−179.1
HC5A—C5A—C6A—HC6A	0.9
P1A—C7A—C8A—C9A	−175.7 (3)
P1A—C7A—C8A—HC8A	4.3
C12A—C7A—C8A—C9A	1.7 (6)
C12A—C7A—C8A—HC8A	−178.3
P1A—C7A—C12A—C11A	176.6 (3)
P1A—C7A—C12A—HC12A	−3.4
C8A—C7A—C12A—C11A	−0.8 (6)
C8A—C7A—C12A—HC12A	179.2
C7A—C8A—C9A—C10A	−1.6 (7)
C7A—C8A—C9A—HC9A	178.4
HC8A—C8A—C9A—C10A	178.4
HC8A—C8A—C9A—HC9A	−1.6
C8A—C9A—C10A—C11A	0.7 (7)
C8A—C9A—C10A—HC10A	−179.3
HC9A—C9A—C10A—C11A	−179.3
HC9A—C9A—C10A—HC10A	0.7
C9A—C10A—C11A—C12A	0.2 (7)
C9A—C10A—C11A—HC11A	−179.8
HC10A—C10A—C11A—C12A	−179.8
P1B—C1B—C2B—HC2B	−2.2
C6B—C1B—C2B—C3B	−3.2 (6)
C6B—C1B—C2B—HC2B	176.8
P1B—C1B—C6B—C5B	−179.2 (3)
P1B—C1B—C6B—HC6B	0.8
C2B—C1B—C6B—C5B	1.8 (6)
C2B—C1B—C6B—HC6B	−178.2
C1B—C2B—C3B—C4B	2.6 (7)
C1B—C2B—C3B—HC3B	−177.4
HC2B—C2B—C3B—C4B	−177.4
HC2B—C2B—C3B—HC3B	2.6
C2B—C3B—C4B—C5B	−0.7 (8)
C2B—C3B—C4B—HC4B	179.3
HC3B—C3B—C4B—C5B	179.3
HC3B—C3B—C4B—HC4B	−0.7
C3B—C4B—C5B—C6B	−0.7 (7)
C3B—C4B—C5B—HC5B	179.3
HC4B—C4B—C5B—C6B	179.3
HC4B—C4B—C5B—HC5B	−0.7
C4B—C5B—C6B—C1B	0.2 (6)
C4B—C5B—C6B—HC6B	−179.8
HC5B—C5B—C6B—C1B	−179.8
HC5B—C5B—C6B—HC6B	0.2
P1B—C7B—C8B—C9B	175.9 (3)
P1B—C7B—C8B—HC8B	−4.1
C12B—C7B—C8B—C9B	−0.4 (6)
C12B—C7B—C8B—HC8B	179.6
P1B—C7B—C12B—C11B	−175.0 (3)
P1B—C7B—C12B—HC12B	5.0
C8B—C7B—C12B—C11B	1.3 (6)
C8B—C7B—C12B—HC12B	−178.7
C7B—C8B—C9B—C10B	−0.6 (6)
C7B—C8B—C9B—HC9B	179.4
HC8B—C8B—C9B—C10B	179.4
HC8B—C8B—C9B—HC9B	−0.6
C8B—C9B—C10B—C11B	0.7 (6)
C8B—C9B—C10B—HC10B	−179.3
HC9B—C9B—C10B—C11B	−179.3
HC9B—C9B—C10B—HC10B	0.7
C9B—C10B—C11B—C12B	0.2 (6)
C9B—C10B—C11B—HC11B	−179.8
HC10B—C10B—C11B—C12B	−179.8
HC10B—C10B—C11B—HC11B	0.2
C10B—C11B—C12B—C7B	−1.2 (6)
C10B—C11B—C12B—HC12B	178.8
HC11B—C11B—C12B—C7B	178.8
HC11B—C11B—C12B—HC12B	−1.2
P1B—C13B—C14B—C15B	177.7 (3)

HC10A—C10A—C11A—HC11A	0.2
C10A—C11A—C12A—C7A	−0.2 (6)
C10A—C11A—C12A—HC12A	179.8
HC11A—C11A—C12A—C7A	179.8
HC11A—C11A—C12A—HC12A	−0.2
P1A—C13A—C14A—C15A	−178.4 (3)
P1A—C13A—C14A—HC14A	1.6
C18A—C13A—C14A—C15A	−0.5 (6)
C18A—C13A—C14A—HC14A	179.5
P1A—C13A—C18A—C17A	177.2 (3)
P1A—C13A—C18A—HC18A	−2.8
C14A—C13A—C18A—C17A	−0.8 (6)
C14A—C13A—C18A—HC18A	179.2
C13A—C14A—C15A—C16A	1.7 (7)
C13A—C14A—C15A—HC15A	−178.3
HC14A—C14A—C15A—C16A	−178.3
HC14A—C14A—C15A—HC15A	1.7
C14A—C15A—C16A—C17A	−1.5 (7)
C14A—C15A—C16A—HC16A	178.5
HC15A—C15A—C16A—C17A	178.5
HC15A—C15A—C16A—HC16A	−1.5
C15A—C16A—C17A—C18A	0.3 (7)
C15A—C16A—C17A—HC17A	−179.7
HC16A—C16A—C17A—C18A	−179.7
HC16A—C16A—C17A—HC17A	0.3
C16A—C17A—C18A—C13A	0.9 (6)
C16A—C17A—C18A—HC18A	−179.1
HC17A—C17A—C18A—C13A	−179.1
HC17A—C17A—C18A—HC18A	0.9
P1A—C19A—C20A—C21A	178.5 (3)
P1A—C19A—C20A—HC20A	−1.5
C24A—C19A—C20A—C21A	0.9 (6)
C24A—C19A—C20A—HC20A	−179.1
P1A—C19A—C24A—C23A	−178.7 (3)
P1A—C19A—C24A—HC24A	1.3
C20A—C19A—C24A—C23A	−1.2 (6)
C20A—C19A—C24A—HC24A	178.8
C19A—C20A—C21A—C22A	0.1 (7)
C19A—C20A—C21A—HC21A	−179.9
HC20A—C20A—C21A—C22A	−179.9
HC20A—C20A—C21A—HC21A	0.1
C20A—C21A—C22A—C23A	−0.8 (7)
C20A—C21A—C22A—HC22A	179.2
HC21A—C21A—C22A—C23A	179.2
HC21A—C21A—C22A—HC22A	−0.8
C21A—C22A—C23A—C24A	0.5 (7)
C21A—C22A—C23A—HC23A	−179.5
HC22A—C22A—C23A—C24A	−179.5
P1B—C13B—C14B—HC14B	−2.3
C18B—C13B—C14B—C15B	0.9 (6)
C18B—C13B—C14B—HC14B	−179.1
P1B—C13B—C18B—C17B	−177.8 (3)
P1B—C13B—C18B—HC18B	2.2
C14B—C13B—C18B—C17B	−0.8 (6)
C14B—C13B—C18B—HC18B	179.2
C13B—C14B—C15B—C16B	−0.3 (7)
C13B—C14B—C15B—HC15B	179.7
HC14B—C14B—C15B—C16B	179.7
HC14B—C14B—C15B—HC15B	−0.3
C14B—C15B—C16B—C17B	−0.3 (7)
C14B—C15B—C16B—HC16B	179.7
HC15B—C15B—C16B—C17B	179.7
HC15B—C15B—C16B—HC16B	−0.3
C15B—C16B—C17B—C18B	0.4 (7)
C15B—C16B—C17B—HC17B	−179.6
HC16B—C16B—C17B—C18B	−179.6
HC16B—C16B—C17B—HC17B	0.4
C16B—C17B—C18B—C13B	0.2 (6)
C16B—C17B—C18B—HC18B	−179.8
HC17B—C17B—C18B—C13B	−179.8
HC17B—C17B—C18B—HC18B	0.2
P1B—C19B—C20B—C21B	179.2 (3)
P1B—C19B—C20B—HC20B	−0.8
C24B—C19B—C20B—C21B	−0.7 (6)
C24B—C19B—C20B—HC20B	179.3
P1B—C19B—C24B—C23B	−178.9 (3)
P1B—C19B—C24B—HC24B	1.1
C20B—C19B—C24B—C23B	0.9 (6)
C20B—C19B—C24B—HC24B	−179.1
C19B—C20B—C21B—C22B	−0.4 (6)
C19B—C20B—C21B—HC21B	179.6
HC20B—C20B—C21B—C22B	179.6
HC20B—C20B—C21B—HC21B	−0.4
C20B—C21B—C22B—C23B	1.2 (7)
C20B—C21B—C22B—HC22B	−178.8
HC21B—C21B—C22B—C23B	−178.8
HC21B—C21B—C22B—HC22B	1.2
C21B—C22B—C23B—C24B	−1.0 (7)
C21B—C22B—C23B—HC23B	179.0
HC22B—C22B—C23B—C24B	179.0
HC22B—C22B—C23B—HC23B	−1.0
C22B—C23B—C24B—C19B	−0.1 (7)
C22B—C23B—C24B—HC24B	179.9
HC23B—C23B—C24B—C19B	179.9
HC23B—C23B—C24B—HC24B	−0.1
H1O4C—O4C—C2C—O3C	2.2

HC22A—C22A—C23A—HC23A	0.5	H1O4C—O4C—C2C—C1C	−177.3
C22A—C23A—C24A—C19A	0.4 (6)	O1C—C1C—C2C—O3C	−71.5 (5)
C22A—C23A—C24A—HC24A	−179.6	O1C—C1C—C2C—O4C	108.0 (4)
HC23A—C23A—C24A—C19A	−179.6	O2C—C1C—C2C—O3C	106.9 (5)
HC23A—C23A—C24A—HC24A	0.4	O2C—C1C—C2C—O4C	−73.6 (5)
C7B—P1B—C1B—C2B	178.9 (3)	H1O4D—O4D—C2D—O3D	−2.6
C7B—P1B—C1B—C6B	−0.1 (4)	H1O4D—O4D—C2D—C1D	175.1
C13B—P1B—C1B—C2B	−63.4 (4)	O1D—C1D—C2D—O3D	−82.3 (6)
C13B—P1B—C1B—C6B	117.6 (3)	O1D—C1D—C2D—O4D	99.8 (5)
C19B—P1B—C1B—C2B	58.5 (4)	O2D—C1D—C2D—O3D	95.8 (5)
C19B—P1B—C1B—C6B	−120.5 (3)	O2D—C1D—C2D—O4D	−82.0 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4*C*—H1*O*4*C*···O1*D*	1.00	1.51	2.505 (2)	180
O4*D*—H1*O*4*D*···O1*C*^{i}	1.00	1.50	2.500 (2)	180

Symmetry code: (i) *x*, *y*−1, *z*.