Crystal structure of (1*S*,2*R*,3*R*,5*aR*,6*S*,7*R*,8*R*,10*aR*)-5,10-di-(*tert*-butoxy-carbonyl)-3,8-di-(iodomethyl)-1,2:6,7-di-isopropylidenedioxy-perhydro-dipyrrolo[1,2-*b*:1,2-*e*]-1,2,4,5-tetrazine, C₂₆H₄₂I₂N₄O₈

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Abstract

C₂₆H₄₂I₂N₄O₈, orthorhombic, *P*2₁2₁2₁ (No. 19), *a* = 14.742(2) Å, *b* = 21.389(3) Å, *c* = 22.688(3) Å, *V* = 7153.9 Å³, *Z* = 8, *R*_{gt}(*F*) = 0.067, *wR*_{all}(*F*²) = 0.136, *T* = 293 K.

Source of material

The title compound has been obtained by iodocyclisation of *N*-(*tert*-butoxycarbonyl)-2,3-isopropylidene-D-erythro-4-pentosehydrazone and iodine in acetonitrile using NaHCO₃ as base [1,2]. After hydrolysis and MPLC separation two stereoisomeric dimers (d. r. = 3:2) were isolated. The major isomer was obtained in the form of yellow crystals by crystallization from isopropanol (mp 436 K – 437 K, [*α*]₂₀^D = +67.3 (*c* = 1.26, CHCl₃)).

Discussion

The compound crystallizes with two molecules in the asymmetric unit. In the *ab* projection of the packing diagram, we observe layer-like orientations of the molecules along the *b*-axis. The iodine atoms work as distance holder between these layers.

Table 1. Data collection and handling.

Crystal:	yellow block, size 0.3 × 0.3 × 0.5 mm
Wavelength:	Mo K _α radiation (0.71073 Å)
μ:	18.03 cm ⁻¹
Diffractometer, scan mode:	Nicolet P3, Wyckoff
2θ _{max} :	50°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	6906, 6906
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 4042
<i>N</i> (<i>param</i>) _{refined} :	722
Programs:	SHELXS-86 [3], SHELXL-93 [4], SHELXTL-plus [5]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(2A)	4a	0.125(1)	0.5012(7)	0.3778(7)	0.066
H(3A)	4a	0.112(1)	0.6087(9)	0.4409(7)	0.078
H(7A)	4a	0.0733(9)	0.6814(8)	0.3748(7)	0.064
H(8A)	4a	0.1975(9)	0.6572(7)	0.3222(6)	0.059
H(11A)	4a	0.379(1)	0.5266(8)	0.3223(7)	0.066
H(13A)	4a	0.272(1)	0.6557(7)	0.4117(7)	0.067
H(14A)	4a	0.388(1)	0.7036(7)	0.3642(6)	0.066
H(18A)	4a	0.346(1)	0.6470(8)	0.2836(6)	0.079
H(22A)	4a	0.273(2)	0.374(1)	0.229(1)	0.256
H(22B)	4a	0.196(2)	0.327(1)	0.212(1)	0.256
H(22C)	4a	0.199(2)	0.355(1)	0.276(1)	0.256
H(23A)	4a	0.138(2)	0.468(1)	0.1392(8)	0.180
H(23B)	4a	0.166(2)	0.399(1)	0.1252(8)	0.180
H(23C)	4a	0.239(2)	0.447(1)	0.1484(8)	0.180
H(24A)	4a	0.025(2)	0.443(1)	0.207(1)	0.226
H(24B)	4a	0.040(2)	0.400(1)	0.262(1)	0.226
H(24C)	4a	0.037(2)	0.371(1)	0.198(1)	0.226
H(28A)	4a	0.373(2)	0.452(1)	0.558(1)	0.247
H(28B)	4a	0.375(2)	0.379(1)	0.560(1)	0.247
H(28C)	4a	0.286(2)	0.414(1)	0.542(1)	0.247
H(29A)	4a	0.501(2)	0.459(1)	0.493(1)	0.231
H(29B)	4a	0.499(2)	0.428(1)	0.430(1)	0.231
H(29C)	4a	0.513(2)	0.387(1)	0.487(1)	0.231
H(30A)	4a	0.369(2)	0.3608(9)	0.403(1)	0.240
H(30B)	4a	0.284(2)	0.3566(9)	0.444(1)	0.240
H(30C)	4a	0.373(2)	0.3214(9)	0.462(1)	0.240
H(31A)	4a	0.063(1)	0.6194(7)	0.2418(6)	0.087
H(31B)	4a	0.165(1)	0.6240(7)	0.2243(6)	0.087
H(32A)	4a	0.420(1)	0.6059(7)	0.4757(6)	0.067
H(32B)	4a	0.319(1)	0.6015(7)	0.4978(6)	0.067
H(33A)	4a	-0.177(1)	0.572(1)	0.4180(9)	0.208
H(33B)	4a	-0.189(1)	0.616(1)	0.3631(9)	0.208
H(33C)	4a	-0.137(1)	0.640(1)	0.4191(9)	0.208
H(34A)	4a	-0.102(2)	0.491(1)	0.354(1)	0.204
H(34B)	4a	-0.011(2)	0.508(1)	0.322(1)	0.204
H(34C)	4a	-0.104(2)	0.533(1)	0.298(1)	0.204

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Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(35A)	4a	0.621(1)	0.557(1)	0.3100(9)	0.190
H(35B)	4a	0.546(1)	0.533(1)	0.3538(9)	0.190
H(35C)	4a	0.628(1)	0.573(1)	0.3773(9)	0.190
H(36A)	4a	0.629(1)	0.667(1)	0.2822(9)	0.215
H(36B)	4a	0.636(1)	0.689(1)	0.3481(9)	0.215
H(36C)	4a	0.559(1)	0.715(1)	0.3078(9)	0.215
H(2B)	4a	0.820(1)	0.5364(6)	0.6867(6)	0.054
H(3B)	4a	0.994(1)	0.5011(8)	0.7176(7)	0.077
H(7B)	4a	1.079(1)	0.5790(8)	0.6759(7)	0.076
H(8B)	4a	1.023(1)	0.5434(7)	0.5875(6)	0.058
H(11B)	4a	0.815(1)	0.4373(6)	0.5413(7)	0.066
H(13B)	4a	1.036(1)	0.4437(9)	0.6172(6)	0.079
H(14B)	4a	1.072(1)	0.4127(9)	0.5246(7)	0.086
H(18B)	4a	0.974(1)	0.4836(7)	0.4951(7)	0.069
H(22D)	4a	0.590(1)	0.574(1)	0.6201(9)	0.159
H(22E)	4a	0.588(1)	0.547(1)	0.5561(9)	0.159
H(22F)	4a	0.525(1)	0.603(1)	0.5728(9)	0.159
H(23D)	4a	0.650(1)	0.6100(9)	0.4734(7)	0.131
H(23E)	4a	0.702(1)	0.6722(9)	0.4865(7)	0.131
H(23F)	4a	0.596(1)	0.6705(9)	0.4908(7)	0.131
H(24D)	4a	0.663(1)	0.6747(9)	0.6396(8)	0.160
H(24E)	4a	0.604(1)	0.7104(9)	0.5930(8)	0.160
H(24F)	4a	0.710(1)	0.7121(9)	0.5888(8)	0.160
H(28D)	4a	0.668(1)	0.351(1)	0.746(1)	0.171

Table 2. Continued.

Atom	Site	x	y	z	U _{iso}
H(28E)	4a	0.731(1)	0.293(1)	0.736(1)	0.171
H(28F)	4a	0.626(1)	0.287(1)	0.725(1)	0.171
H(29D)	4a	0.717(2)	0.291(1)	0.580(1)	0.330
H(29E)	4a	0.657(2)	0.250(1)	0.622(1)	0.330
H(29F)	4a	0.761(2)	0.255(1)	0.633(1)	0.330
H(30D)	4a	0.606(2)	0.410(1)	0.664(1)	0.252
H(30E)	4a	0.557(2)	0.352(1)	0.636(1)	0.252
H(30F)	4a	0.626(2)	0.391(1)	0.598(1)	0.252
H(31C)	4a	0.943(1)	0.6645(7)	0.5870(7)	0.083
H(31D)	4a	0.958(1)	0.6238(7)	0.5302(7)	0.083
H(32C)	4a	0.980(2)	0.322(1)	0.6212(9)	0.142
H(32D)	4a	0.997(2)	0.364(1)	0.6766(9)	0.142
H(33D)	4a	1.013(2)	0.707(1)	0.7870(7)	0.177
H(33E)	4a	1.062(2)	0.642(1)	0.7903(7)	0.177
H(33F)	4a	0.979(2)	0.656(1)	0.8313(7)	0.177
H(34D)	4a	0.861(2)	0.713(1)	0.734(1)	0.232
H(34E)	4a	0.818(2)	0.663(1)	0.777(1)	0.232
H(34F)	4a	0.821(2)	0.651(1)	0.708(1)	0.232
H(35D)	4a	0.841(2)	0.308(1)	0.416(1)	0.310
H(35E)	4a	0.824(2)	0.312(1)	0.484(1)	0.310
H(35F)	4a	0.891(2)	0.262(1)	0.459(1)	0.310
H(36D)	4a	0.979(2)	0.349(1)	0.3751(9)	0.198
H(36E)	4a	1.041(2)	0.306(1)	0.4139(9)	0.198
H(36F)	4a	1.053(2)	0.379(1)	0.4165(9)	0.198

Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
I(1A)	4a	0.1021(1)	0.73791(6)	0.23047(7)	0.099(1)	0.097(1)	0.114(1)	-0.0134(9)	-0.022(1)	0.0429(9)
I(2A)	4a	0.37399(8)	0.71732(5)	0.51610(5)	0.0692(7)	0.0688(7)	0.0759(7)	-0.0019(7)	0.0010(7)	-0.0116(6)
N(1A)	4a	0.2398(9)	0.5356(7)	0.4114(6)	0.053(9)	0.07(1)	0.062(9)	-0.007(8)	-0.013(8)	0.018(8)
C(2A)	4a	0.154(1)	0.5422(7)	0.3797(7)	0.06(1)	0.05(1)	0.05(1)	-0.009(9)	0.001(9)	-0.002(8)
C(3A)	4a	0.086(1)	0.5893(9)	0.4055(7)	0.05(1)	0.10(1)	0.041(9)	0.00(1)	0.003(8)	-0.01(1)
O(4A)	4a	0.0000(8)	0.5656(6)	0.4184(5)	0.057(8)	0.11(1)	0.066(8)	0.002(8)	0.011(6)	0.029(8)
C(5A)	4a	-0.062(1)	0.580(1)	0.3703(8)	0.06(1)	0.11(2)	0.05(1)	-0.00(1)	-0.01(1)	0.01(1)
O(6A)	4a	-0.0153(8)	0.6243(7)	0.3351(6)	0.050(8)	0.13(1)	0.10(1)	0.002(8)	0.014(7)	0.055(9)
C(7A)	4a	0.0721(9)	0.6392(8)	0.3579(7)	0.030(9)	0.07(1)	0.06(1)	-0.009(8)	0.011(8)	0.000(9)
C(8A)	4a	0.1451(9)	0.6310(7)	0.3123(6)	0.033(9)	0.07(1)	0.049(9)	0.005(8)	0.008(7)	0.007(8)
N(9A)	4a	0.1687(8)	0.5642(6)	0.3205(5)	0.036(7)	0.059(9)	0.046(8)	-0.001(7)	0.002(6)	-0.007(7)
N(10A)	4a	0.2506(9)	0.5458(6)	0.2941(6)	0.045(8)	0.07(1)	0.057(9)	0.005(7)	-0.003(7)	-0.012(7)
C(11A)	4a	0.336(1)	0.5613(8)	0.3263(7)	0.05(1)	0.06(1)	0.05(1)	-0.014(9)	-0.012(9)	0.015(9)
N(12A)	4a	0.3132(9)	0.5699(7)	0.3892(5)	0.063(9)	0.07(1)	0.040(8)	-0.006(8)	-0.013(7)	0.007(7)
C(13A)	4a	0.328(1)	0.6316(7)	0.4129(7)	0.040(9)	0.06(1)	0.07(1)	-0.014(8)	0.011(8)	0.003(9)
C(14A)	4a	0.396(1)	0.6584(7)	0.3692(6)	0.05(1)	0.06(1)	0.050(9)	0.006(9)	0.006(8)	0.009(8)
O(15A)	4a	0.4840(8)	0.6423(6)	0.3849(5)	0.046(7)	0.14(1)	0.053(7)	-0.012(7)	0.005(6)	-0.030(7)
C(16A)	4a	0.534(1)	0.626(1)	0.3349(8)	0.05(1)	0.12(2)	0.07(1)	-0.02(1)	-0.02(1)	-0.00(1)
O(17A)	4a	0.4698(8)	0.6147(7)	0.2879(5)	0.051(8)	0.16(1)	0.052(7)	-0.023(8)	0.018(6)	-0.018(8)
C(18A)	4a	0.383(1)	0.6226(8)	0.3109(6)	0.07(1)	0.10(1)	0.036(8)	0.00(1)	0.002(9)	-0.002(9)
C(19A)	4a	0.252(1)	0.4929(9)	0.2594(8)	0.06(1)	0.08(1)	0.07(1)	0.01(1)	0.00(1)	-0.03(1)
O(19A)	4a	0.3213(9)	0.4737(7)	0.2391(6)	0.075(9)	0.13(1)	0.09(1)	0.009(9)	0.005(8)	-0.065(9)
O(20A)	4a	0.1694(8)	0.4708(6)	0.2516(5)	0.052(7)	0.097(9)	0.071(8)	0.005(7)	-0.017(6)	-0.030(7)
C(21A)	4a	0.154(1)	0.4150(9)	0.2159(9)	0.08(1)	0.08(1)	0.08(1)	-0.00(1)	-0.03(1)	-0.03(1)
C(22A)	4a	0.210(2)	0.363(1)	0.235(1)	0.21(3)	0.09(2)	0.21(3)	-0.01(2)	-0.10(3)	-0.00(2)
C(23A)	4a	0.176(2)	0.434(1)	0.1509(8)	0.15(2)	0.14(2)	0.07(1)	-0.02(2)	-0.02(2)	-0.05(2)
C(24A)	4a	0.055(2)	0.407(1)	0.221(1)	0.11(2)	0.18(3)	0.16(3)	-0.06(2)	-0.03(2)	-0.07(2)
O(25A)	4a	0.1965(9)	0.4457(6)	0.4553(6)	0.08(1)	0.10(1)	0.11(1)	-0.022(9)	-0.009(9)	0.044(9)
C(25A)	4a	0.256(1)	0.4801(9)	0.4398(8)	0.05(1)	0.08(1)	0.08(1)	0.00(1)	-0.02(1)	0.01(1)
O(26A)	4a	0.3455(8)	0.4715(5)	0.4483(6)	0.073(9)	0.059(7)	0.11(1)	-0.004(6)	-0.012(8)	0.033(7)
C(27A)	4a	0.380(2)	0.414(1)	0.4761(9)	0.12(2)	0.09(2)	0.09(2)	0.03(2)	-0.05(2)	-0.00(1)
C(28A)	4a	0.351(2)	0.415(1)	0.540(1)	0.19(3)	0.18(3)	0.13(2)	0.04(2)	-0.04(2)	0.05(2)
C(29A)	4a	0.483(2)	0.423(1)	0.471(1)	0.12(2)	0.11(2)	0.24(3)	0.01(2)	-0.06(2)	0.04(2)
C(30A)	4a	0.349(2)	0.3583(9)	0.443(1)	0.20(3)	0.07(1)	0.22(3)	0.01(2)	-0.04(3)	-0.03(2)
C(31A)	4a	0.119(1)	0.6413(7)	0.2499(6)	0.06(1)	0.10(1)	0.06(1)	-0.01(1)	-0.01(1)	-0.004(9)
C(32A)	4a	0.361(1)	0.6267(7)	0.4752(6)	0.05(1)	0.07(1)	0.049(9)	0.000(9)	-0.006(8)	-0.003(8)
C(33A)	4a	-0.149(1)	0.604(1)	0.3948(9)	0.05(1)	0.28(3)	0.10(2)	0.07(2)	0.03(1)	0.05(2)
C(34A)	4a	-0.070(2)	0.523(1)	0.333(1)	0.17(3)	0.12(2)	0.12(2)	0.01(2)	-0.08(2)	0.02(2)
C(35A)	4a	0.587(1)	0.567(1)	0.3449(9)	0.09(2)	0.18(3)	0.10(2)	0.05(2)	-0.03(1)	-0.05(2)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(36A)	4a	0.595(1)	0.679(1)	0.3166(9)	0.11(2)	0.21(3)	0.11(2)	-0.11(2)	0.05(2)	-0.02(2)
I(1B)	4a	1.11600(9)	0.67195(5)	0.55959(5)	0.0829(8)	0.0696(7)	0.0679(7)	-0.0212(8)	0.0072(7)	0.0027(6)
I(2B)	4a	1.1534(1)	0.32525(8)	0.63940(7)	0.099(1)	0.130(1)	0.098(1)	0.052(1)	0.0074(9)	0.026(1)
N(1B)	4a	0.8675(8)	0.4509(5)	0.6590(5)	0.058(8)	0.049(7)	0.042(7)	-0.001(7)	0.022(7)	0.011(6)
C(2B)	4a	0.875(1)	0.5206(6)	0.6684(6)	0.045(9)	0.037(8)	0.054(9)	0.009(8)	0.006(9)	-0.007(7)
C(3B)	4a	0.958(1)	0.5380(8)	0.7069(7)	0.08(1)	0.07(1)	0.05(1)	0.00(1)	0.00(1)	-0.002(9)
O(4B)	4a	0.9318(9)	0.5731(6)	0.7574(5)	0.13(1)	0.09(1)	0.047(7)	-0.027(9)	0.008(7)	0.001(7)
C(5B)	4a	0.943(2)	0.6378(9)	0.7474(8)	0.13(2)	0.07(1)	0.05(1)	-0.01(1)	-0.01(1)	-0.01(1)
O(6B)	4a	0.984(1)	0.6442(6)	0.6915(6)	0.18(2)	0.060(8)	0.062(8)	-0.003(9)	-0.01(1)	0.005(7)
C(7B)	4a	1.013(1)	0.5849(8)	0.6706(7)	0.05(1)	0.07(1)	0.07(1)	-0.02(1)	0.006(9)	0.01(1)
C(8B)	4a	0.985(1)	0.5755(7)	0.6062(6)	0.05(1)	0.05(1)	0.05(1)	0.007(8)	-0.001(8)	0.009(8)
N(9B)	4a	0.8912(9)	0.5530(5)	0.6130(5)	0.066(9)	0.045(7)	0.036(7)	0.003(7)	-0.011(7)	0.015(6)
N(10B)	4a	0.8500(8)	0.5248(5)	0.5650(5)	0.049(8)	0.051(7)	0.048(7)	0.004(6)	-0.007(7)	-0.011(6)
C(11B)	4a	0.871(1)	0.4584(6)	0.5535(7)	0.07(1)	0.033(8)	0.06(1)	-0.007(8)	0.01(1)	-0.010(7)
N(12B)	4a	0.9046(9)	0.4285(6)	0.6070(5)	0.07(1)	0.060(8)	0.050(8)	0.026(8)	0.026(7)	0.017(7)
C(13B)	4a	0.997(1)	0.4094(9)	0.6032(6)	0.06(1)	0.09(1)	0.04(1)	0.04(1)	0.027(9)	0.013(9)
C(14B)	4a	1.010(1)	0.4024(9)	0.5363(7)	0.07(1)	0.10(2)	0.04(1)	0.02(1)	0.003(9)	0.02(1)
O(15B)	4a	0.984(1)	0.3429(6)	0.5152(6)	0.24(2)	0.058(9)	0.066(9)	0.02(1)	0.02(1)	-0.003(8)
C(16B)	4a	0.944(2)	0.348(1)	0.4599(9)	0.14(2)	0.07(2)	0.06(1)	-0.00(1)	0.04(1)	-0.01(1)
O(17B)	4a	0.910(1)	0.4103(7)	0.4593(5)	0.14(1)	0.12(1)	0.067(9)	0.04(1)	-0.019(8)	-0.022(8)
C(18B)	4a	0.944(1)	0.4449(7)	0.5081(7)	0.08(1)	0.05(1)	0.038(9)	-0.001(9)	-0.021(9)	0.003(8)
C(19B)	4a	0.766(1)	0.5468(7)	0.5471(7)	0.07(1)	0.05(1)	0.05(1)	-0.014(9)	-0.010(9)	0.000(8)
O(19B)	4a	0.7237(8)	0.5191(5)	0.5105(5)	0.073(8)	0.057(7)	0.093(9)	0.010(6)	-0.019(8)	-0.020(7)
O(20B)	4a	0.7457(7)	0.6002(5)	0.5726(5)	0.060(7)	0.053(7)	0.070(8)	0.014(6)	-0.020(6)	-0.016(6)
C(21B)	4a	0.657(1)	0.6294(8)	0.5607(7)	0.06(1)	0.08(1)	0.05(1)	0.01(1)	0.00(1)	-0.01(1)
C(22B)	4a	0.583(1)	0.584(1)	0.5791(9)	0.08(2)	0.12(2)	0.11(2)	0.03(1)	0.02(1)	0.02(2)
C(23B)	4a	0.651(1)	0.6471(9)	0.4972(7)	0.08(1)	0.11(2)	0.08(1)	0.03(1)	-0.01(1)	-0.01(1)
C(24B)	4a	0.659(1)	0.6868(9)	0.5990(8)	0.10(2)	0.10(2)	0.11(2)	0.07(1)	-0.03(1)	-0.05(1)
C(25B)	4a	0.787(1)	0.4240(8)	0.6790(8)	0.07(1)	0.06(1)	0.06(1)	-0.01(1)	0.02(1)	-0.01(1)
O(25B)	4a	0.7403(8)	0.4452(6)	0.7156(6)	0.071(8)	0.10(1)	0.09(1)	-0.015(7)	0.045(8)	-0.024(8)
O(26B)	4a	0.7752(8)	0.3699(6)	0.6513(5)	0.090(9)	0.074(9)	0.084(9)	-0.038(7)	0.033(8)	-0.021(7)
C(27B)	4a	0.692(2)	0.333(1)	0.659(1)	0.09(2)	0.11(2)	0.12(2)	-0.06(2)	0.01(1)	-0.01(2)
C(28B)	4a	0.678(1)	0.315(1)	0.722(1)	0.07(1)	0.12(2)	0.15(2)	-0.04(1)	0.03(2)	0.01(2)
C(29B)	4a	0.708(2)	0.277(1)	0.620(1)	0.22(3)	0.15(3)	0.29(4)	-0.11(3)	0.08(3)	-0.13(3)
C(30B)	4a	0.613(2)	0.376(1)	0.637(1)	0.11(2)	0.23(3)	0.16(3)	-0.04(2)	-0.05(2)	0.08(2)
C(31B)	4a	0.983(1)	0.6338(7)	0.5688(7)	0.09(1)	0.06(1)	0.06(1)	-0.01(1)	-0.02(1)	0.010(9)
C(32B)	4a	1.017(2)	0.356(1)	0.6364(9)	0.17(2)	0.11(2)	0.08(2)	0.06(2)	0.00(2)	0.02(1)
C(33B)	4a	1.005(2)	0.663(1)	0.7930(7)	0.17(2)	0.12(2)	0.06(1)	-0.06(2)	-0.04(1)	-0.01(1)
C(34B)	4a	0.853(2)	0.669(1)	0.741(1)	0.13(2)	0.12(2)	0.22(3)	0.05(2)	0.02(2)	0.04(2)
C(35B)	4a	0.868(2)	0.304(1)	0.455(1)	0.25(4)	0.19(3)	0.18(3)	-0.14(3)	0.02(3)	-0.03(2)
C(36B)	4a	1.010(2)	0.345(1)	0.4123(9)	0.14(2)	0.16(2)	0.10(2)	0.03(2)	0.03(2)	-0.05(2)

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