```
# Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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_publ_contact_author_name        'Tor, Yitzhak '
_publ_contact_author_email       ytor@ucsd.edu

_publ_section_title
;
Fluorescent nucleoside analogue
displays enhanced emission upon pairing with guanine
;
loop_
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'Yu Xie'
T.Maxson
Y.Tor

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N N 0.0311 0.0180 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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'x+1/2, -y+1/2, -z'
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2^, conventional R-factors R are based
on F, with F set to zero for negative F^2^. The threshold expression of
F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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H2 H 0.6483 0.9198 0.1140 0.022 Uiso 1 1 calc R . .
C3 C 0.6346(3) 0.72544(19) 0.11803(11) 0.0188(4) Uani 1 1 d . . .
C4 C 0.6201(3) 0.61478(19) 0.07447(12) 0.0195(4) Uani 1 1 d . . .
H4 H 0.6173 0.5325 0.0961 0.023 Uiso 1 1 calc R . .
C5 C 0.6100(3) 0.62722(19) 0.00076(12) 0.0180(4) Uani 1 1 d . . .
H5 H 0.6000 0.5525 -0.0281 0.022 Uiso 1 1 calc R . .
C6 C 0.6140(3) 0.7467(2) -0.03308(11) 0.0166(4) Uani 1 1 d . . .
C7 C 0.6088(3) 0.75658(18) -0.11061(11) 0.0163(4) Uani 1 1 d . . .
C8 C 0.6319(3) 0.98927(18) -0.09770(11) 0.0157(4) Uani 1 1 d . . .
C9 C 0.6385(3) 1.09785(19) 0.01676(11) 0.0167(4) Uani 1 1 d . . .
H101 H 0.6432 1.1700 -0.0186 0.020 Uiso 1 1 calc R . .
C10 C 0.4722(3) 1.1238(2) 0.07060(12) 0.0199(5) Uani 1 1 d . . .
H10A H 0.3708 1.1793 0.0489 0.024 Uiso 1 1 calc R . .
H10B H 0.4106 1.0430 0.0867 0.024 Uiso 1 1 calc R . .
C11 C 0.5747(3) 1.19108(18) 0.13362(11) 0.0162(4) Uani 1 1 d . . .
H11 H 0.5567 1.1414 0.1793 0.019 Uiso 1 1 calc R . .
C12 C 0.7923(3) 1.19400(19) 0.11207(11) 0.0159(4) Uani 1 1 d . . .
H12 H 0.8231 1.2794 0.0907 0.019 Uiso 1 1 calc R . .
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H13B H 0.9390 1.2404 0.2060 0.022 Uiso 1 1 calc R . .
N1 N 0.6187(3) 0.87971(15) -0.13737(9) 0.0170(4) Uani 1 1 d . . .
H1 H 0.6162 0.8883 -0.1847 0.020 Uiso 1 1 calc R . .
N2 N 0.6296(3) 0.97765(15) -0.02370(9) 0.0158(4) Uani 1 1 d . . .
N3 N 0.6475(3) 0.71563(17) 0.19058(10) 0.0235(4) Uani 1 1 d . . .
H3A H 0.6579 0.7849 0.2172 0.028 Uiso 1 1 calc R . .
H3B H 0.6454 0.6400 0.2112 0.028 Uiso 1 1 calc R . .
O1 O 0.5974(2) 0.66558(13) -0.15316(8) 0.0205(3) Uani 1 1 d . . .
O2 O 0.6430(2) 1.09320(12) -0.12922(8) 0.0188(3) Uani 1 1 d . . .
O3 O 0.8156(2) 1.09857(13) 0.05751(8) 0.0176(3) Uani 1 1 d . . .
O4 O 0.5152(2) 1.32051(13) 0.14379(9) 0.0248(4) Uani 1 1 d . . .
H4A H 0.3937 1.3263 0.1379 0.037 Uiso 1 1 calc R . .
O5 O 0.8867(2) 1.05415(13) 0.21191(8) 0.0193(3) Uani 1 1 d . . .
H5A H 0.9394 0.9905 0.1923 0.029 Uiso 1 1 calc R . .
O6 O 0.6307(3) 0.46609(14) 0.26130(9) 0.0247(4) Uani 1 1 d . . .
H6B H 0.611(4) 0.413(2) 0.2242(15) 0.037 Uiso 1 1 d . . .
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C3 0.0174(10) 0.0189(10) 0.0202(11) -0.0007(9) 0.0019(9) 0.0003(9)
C4 0.0194(10) 0.0144(9) 0.0246(11) 0.0038(8) 0.0009(9) -0.0010(9)
C5 0.0185(10) 0.0156(10) 0.0200(10) -0.0016(8) 0.0027(9) -0.0004(9)
C6 0.0159(10) 0.0158(10) 0.0181(10) 0.0003(8) 0.0015(8) -0.0007(9)
C7 0.0158(10) 0.0149(9) 0.0182(10) -0.0020(9) -0.0010(8) -0.0002(8)
C8 0.0151(10) 0.0150(10) 0.0169(10) -0.0006(8) -0.0007(8) -0.0005(9)
C9 0.0212(11) 0.0146(10) 0.0143(9) -0.0003(8) -0.0011(9) -0.0016(9)
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C11 0.0205(11) 0.0102(9) 0.0178(10) -0.0013(8) 0.0024(8) 0.0021(8)
C12 0.0218(11) 0.0132(9) 0.0127(10) -0.0019(8) 0.0016(8) -0.0012(8)
C13 0.0217(11) 0.0161(10) 0.0162(10) -0.0014(9) -0.0003(8) -0.0032(8)
N1 0.0234(9) 0.0168(8) 0.0108(8) -0.0012(7) 0.0012(7) -0.0005(8)
N2 0.0209(9) 0.0117(8) 0.0149(8) -0.0006(7) 0.0009(7) -0.0011(8)
N3 0.0366(11) 0.0165(9) 0.0175(9) 0.0031(7) 0.0013(8) -0.0001(8)
O1 0.0254(8) 0.0172(7) 0.0189(7) -0.0060(6) 0.0020(6) -0.0011(6)
O2 0.0241(8) 0.0152(7) 0.0169(7) 0.0013(6) 0.0000(6) -0.0012(6)
O3 0.0200(8) 0.0173(7) 0.0155(7) -0.0034(6) -0.0014(6) -0.0001(6)
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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.
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C1 C6 1.410(3) . ?
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C2 C3 1.395(3) . ?
C2 H2 0.9500 . ?
C3 N3 1.349(3) . ?
C3 C4 1.415(3) . ?
C4 C5 1.372(3) . ?
C4 H4 0.9500 . ?
C5 C6 1.399(3) . ?
C5 H5 0.9500 . ?
C6 C7 1.439(3) . ?
C7 O1 1.238(2) . ?
C7 N1 1.383(2) . ?
C8 O2 1.237(2) . ?
C8 N1 1.365(2) . ?
C8 N2 1.375(2) . ?
C9 O3 1.427(3) . ?
C9 N2 1.466(3) . ?
C9 C10 1.536(3) . ?
C9 H101 1.0000 . ?
C10 C11 1.532(3) . ?
C10 H10A 0.9900 . ?
C10 H10B 0.9900 . ?
C11 O4 1.427(2) . ?
C11 C12 1.541(3) . ?
C11 H11 1.0000 . ?
C12 O3 1.429(3) . ?
C12 C13 1.516(3) . ?
C12 H12 1.0000 . ?
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C13 O5 1.427(2) . ?
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N3 H3A 0.8800 . ?
N3 H3B 0.8800 . ?
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N3 C3 C2 120.20(18) . . ?
N3 C3 C4 120.60(19) . . ?
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C3 C4 H4 120.3 . . ?
C4 C5 C6 121.94(19) . . ?
C4 C5 H5 119.0 . . ?
C6 C5 H5 119.0 . . ?
C5 C6 C1 118.51(19) . . ?
C5 C6 C7 120.70(19) . . ?
C1 C6 C7 120.79(19) . . ?
O1 C7 N1 119.52(19) . . ?
O1 C7 C6 125.44(19) . . ?
N1 C7 C6 115.04(17) . . ?
O2 C8 N1 119.33(18) . . ?
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N1 C8 N2 117.42(17) . . ?
O3 C9 N2 108.05(17) . . ?
O3 C9 C10 106.55(17) . . ?
N2 C9 C10 116.88(18) . . ?
O3 C9 H101 108.4 . . ?
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C10 C9 H101 108.4 . . ?
C11 C10 C9 103.66(17) . . ?
C11 C10 H10A 111.0 . . ?
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C11 C10 H10B 111.0 . . ?
C9 C10 H10B 111.0 . . ?
H10A C10 H10B 109.0 . . ?
O4 C11 C10 113.99(17) . . ?
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C10 C11 H11 110.3 . . ?
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C11 C12 H12 108.8 . . ?
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C12 C13 H13A 109.1 . . ?
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C12 C13 H13B 109.1 . . ?
H13A C13 H13B 107.9 . . ?
C8 N1 C7 126.46(17) . . ?
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C7 N1 H1 116.8 . . ?
C8 N2 C1 121.63(16) . . ?
C8 N2 C9 115.61(16) . . ?
C1 N2 C9 122.72(16) . . ?
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C3 N3 H3B 120.0 . . ?
H3A N3 H3B 120.0 . . ?
C9 O3 C12 106.39(15) . . ?
C11 O4 H4A 109.5 . . ?
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