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 'x, -y+1/2, z+1/2'

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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
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 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
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 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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O2 O 1.2148(5) 1.4426(2) 0.8823(2) 0.0208(11) Uani 1 1 d . . .
O3 O -0.2417(5) 1.0016(2) 0.4339(2) 0.0223(11) Uani 1 1 d . . .
O4 O -0.4132(6) 1.0110(3) 0.5280(3) 0.0239(11) Uani 1 1 d . . .
O5 O 0.0647(8) 1.1172(3) 0.7783(3) 0.0448(15) Uani 1 1 d . . .
O6 O 0.6672(8) 1.2456(3) 0.5802(3) 0.0499(17) Uani 1 1 d . . .
N1 N 0.5751(6) 1.0889(3) 0.8990(4) 0.0202(12) Uani 1 1 d . . .
N2 N 0.7068(5) 1.1889(2) 0.9128(4) 0.0152(11) Uani 1 1 d . . .
N3 N 0.4184(6) 0.9412(3) 0.7940(3) 0.0148(12) Uani 1 1 d . . .
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N4 N 0.2549(6) 0.9374(3) 0.6968(3) 0.0146(11) Uani 1 1 d . . .
N5 N 0.0737(10) 1.2005(4) 0.6862(4) 0.0408(18) Uani 1 1 d . . .
N6 N 0.5655(8) 1.1639(3) 0.6611(3) 0.0293(14) Uani 1 1 d . . .
C1 C 0.4627(6) 1.1419(3) 0.9121(6) 0.0229(15) Uani 1 1 d . . .
H1 H 0.3511 1.1359 0.9151 0.027 Uiso 1 1 calc R . .
C2 C 0.5439(7) 1.2051(3) 0.9198(5) 0.026(2) Uani 1 1 d . . .
H2 H 0.4987 1.2495 0.9281 0.031 Uiso 1 1 calc R . .
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C7 C 1.0975(7) 1.3319(3) 0.9163(4) 0.0126(14) Uani 1 1 d . . .
C8 C 0.9468(8) 1.3525(3) 0.8877(3) 0.0193(17) Uani 1 1 d . . .
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C9 C 0.8167(7) 1.3056(3) 0.8878(3) 0.0185(16) Uani 1 1 d . . .
H9 H 0.7159 1.3199 0.8702 0.022 Uiso 1 1 calc R . .
C10 C 1.2370(6) 1.3828(3) 0.9118(5) 0.0176(13) Uani 1 1 d . . .
C11 C 0.4854(9) 0.8947(4) 0.7421(3) 0.0246(15) Uani 1 1 d . . .
H11 H 0.5820 0.8699 0.7475 0.029 Uiso 1 1 calc R . .
C12 C 0.3846(8) 0.8920(4) 0.6819(4) 0.0248(16) Uani 1 1 d . . .
H12 H 0.3995 0.8651 0.6392 0.030 Uiso 1 1 calc R . .
C13 C 0.2826(7) 0.9648(3) 0.7655(4) 0.0162(13) Uani 1 1 d . . .
H13 H 0.2137 0.9964 0.7893 0.019 Uiso 1 1 calc R . .
C14 C 0.1220(8) 0.9522(3) 0.6489(4) 0.0177(14) Uani 1 1 d . . .
C15 C 0.1529(8) 0.9639(4) 0.5741(4) 0.0207(15) Uani 1 1 d . . .
H15 H 0.2580 0.9613 0.5556 0.025 Uiso 1 1 calc R . .
C16 C 0.0234(8) 0.9797(3) 0.5269(4) 0.0204(14) Uani 1 1 d . . .
H16 H 0.0424 0.9874 0.4767 0.024 Uiso 1 1 calc R . .
C17 C -0.1340(8) 0.9839(3) 0.5545(4) 0.0169(14) Uani 1 1 d . . .
C18 C -0.1612(8) 0.9729(4) 0.6301(4) 0.0207(14) Uani 1 1 d . . .
H18 H -0.2661 0.9760 0.6487 0.025 Uiso 1 1 calc R . .
C19 C -0.0339(8) 0.9572(3) 0.6783(4) 0.0197(14) Uani 1 1 d . . .
H19 H -0.0524 0.9502 0.7287 0.024 Uiso 1 1 calc R . .
C20 C -0.2725(8) 0.9998(3) 0.5027(4) 0.0209(15) Uani 1 1 d . . .
C21 C 0.0276(14) 1.1527(4) 0.6245(5) 0.061(3) Uani 1 1 d . . .
H21A H 0.0258 1.1788 0.5788 0.091 Uiso 1 1 calc R . .
H21B H -0.0780 1.1334 0.6339 0.091 Uiso 1 1 calc R . .
H21C H 0.1050 1.1149 0.6208 0.091 Uiso 1 1 calc RD . .
C22 C 0.0891(17) 1.2749(5) 0.6661(6) 0.069(3) Uani 1 1 d . . .
H22A H 0.0790 1.2799 0.6132 0.104 Uiso 1 1 calc R . .
H22B H 0.1930 1.2922 0.6816 0.104 Uiso 1 1 calc R . .
H22C H 0.0053 1.3016 0.6902 0.104 Uiso 1 1 calc R . .
C23 C 0.0809(11) 1.1784(5) 0.7574(5) 0.040(2) Uani 1 1 d . . .
H23 H 0.0998 1.2125 0.7936 0.048 Uiso 1 1 calc R . .
C24 C 0.4815(11) 1.0994(5) 0.6765(6) 0.058(3) Uani 1 1 d . . .
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C25 C 0.6452(13) 1.1941(6) 0.7253(5) 0.061(3) Uani 1 1 d . . .
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H25B H 0.6100 1.2421 0.7320 0.091 Uiso 1 1 calc R . .
H25C H 0.7604 1.1932 0.7180 0.091 Uiso 1 1 calc R . .
C26 C 0.5844(10) 1.1930(4) 0.5938(4) 0.0364(19) Uani 1 1 d . . .
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O2 0.019(2) 0.007(2) 0.036(3) 0.0065(19) 0.0019(18) 0.0002(18)
O3 0.023(2) 0.024(3) 0.020(2) 0.006(2) -0.0044(17) -0.003(2)
O4 0.019(3) 0.020(3) 0.033(3) -0.006(2) 0.003(2) 0.008(2)
O5 0.066(4) 0.028(3) 0.041(3) 0.008(3) 0.007(3) 0.006(3)
O6 0.085(5) 0.031(4) 0.033(3) 0.008(3) 0.006(3) -0.009(4)
N1 0.013(2) 0.015(2) 0.033(4) -0.003(3) 0.000(3) -0.0004(19)
N2 0.015(2) 0.008(2) 0.023(3) -0.005(3) 0.001(3) -0.0015(17)
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N6 0.043(4) 0.020(3) 0.025(3) -0.002(3) 0.002(3) -0.005(3)
C1 0.011(3) 0.016(3) 0.041(4) -0.002(5) -0.005(4) -0.001(2)
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C6 0.016(3) 0.009(3) 0.021(3) -0.006(3) 0.000(3) 0.002(3)
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C12 0.027(4) 0.023(4) 0.025(4) -0.003(3) -0.003(3) 0.011(3)
C13 0.024(3) 0.004(3) 0.021(3) -0.001(3) 0.001(3) 0.000(3)
C14 0.023(3) 0.007(3) 0.023(3) -0.006(3) -0.002(3) -0.001(3)
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C20 0.026(4) 0.004(3) 0.032(4) -0.002(3) -0.004(3) -0.004(3)
C21 0.125(10) 0.014(4) 0.042(5) -0.007(4) -0.002(6) -0.004(5)
C22 0.130(10) 0.022(5) 0.055(6) 0.003(5) 0.015(7) -0.005(6)
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C24 0.061(6) 0.037(5) 0.075(7) -0.010(5) 0.030(6) -0.007(5)
C25 0.085(8) 0.064(8) 0.033(5) 0.009(5) -0.009(5) -0.023(6)
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 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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Cd1 O4 2.355(5) 2_575 ?
Cd1 O2 2.361(5) 3_745 ?
Cd1 C10 2.677(5) 3_745 ?
Cd1 C20 2.682(7) 2_575 ?
O1 C10 1.277(7) . ?
O1 Cd1 2.335(4) 3_755 ?
O2 C10 1.262(8) . ?
O2 Cd1 2.361(4) 3_755 ?
O3 C20 1.265(8) . ?
O3 Cd1 2.341(5) 2_574 ?
O4 C20 1.265(8) . ?
O4 Cd1 2.355(5) 2_574 ?
O5 C23 1.222(10) . ?
O6 C26 1.230(10) . ?
N1 C3 1.314(7) . ?
N1 C1 1.385(7) . ?
N2 C3 1.356(7) . ?
N2 C2 1.384(7) . ?
N2 C4 1.423(7) . ?
N3 C13 1.311(8) . ?
N3 C11 1.397(8) . ?
N4 C13 1.360(8) . ?
N4 C12 1.397(8) . ?
N4 C14 1.423(8) . ?
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N5 C22 1.458(11) . ?
N5 C21 1.481(10) . ?
N6 C26 1.340(10) . ?
N6 C24 1.430(11) . ?
N6 C25 1.447(11) . ?
C1 C2 1.376(8) . ?
C4 C9 1.383(9) . ?
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C5 C6 1.385(9) . ?
C6 C7 1.394(9) . ?
C7 C8 1.401(8) . ?
C7 C10 1.503(8) . ?
C8 C9 1.393(9) . ?
C10 Cd1 2.677(5) 3_755 ?
C11 C12 1.367(9) . ?
C14 C15 1.389(9) . ?
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C15 C16 1.397(9) . ?
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C17 C18 1.395(9) . ?
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O2 Cd1 C20 150.51(19) 3_745 2_575 ?
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C10 O2 Cd1 90.0(3) . 3_755 ?
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O2 C10 C7 119.1(5) . . ?
O1 C10 C7 118.3(5) . . ?
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O1 C10 Cd1 60.7(3) . 3_755 ?
C7 C10 Cd1 178.8(6) . 3_755 ?
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C11 C12 N4 107.0(6) . . ?
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C15 C14 N4 118.6(6) . . ?
C19 C14 N4 119.6(6) . . ?
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C16 C17 C18 119.3(6) . . ?
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C14 C19 C18 118.3(6) . . ?
O3 C20 O4 122.2(6) . . ?
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C18 C17 C20 Cd1 -166(14) . . . 2_574 ?
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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
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 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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N2 N 0.4574(3) -0.0986(3) 0.4481(2) 0.0249(9) Uani 1 1 d . . .
N3 N 0.2406(3) 0.0416(3) 0.5980(2) 0.0270(10) Uani 1 1 d . . .
N4 N 0.2436(3) 0.1115(3) 0.6981(2) 0.0269(10) Uani 1 1 d . . .
N5 N 0.5124(4) -0.1807(5) 0.7207(3) 0.0580(18) Uani 1 1 d D . .
O1 O 0.6153(3) -0.4319(3) 0.5166(2) 0.0394(11) Uani 1 1 d D . .
O2 O 0.7210(2) -0.3680(3) 0.4778(2) 0.0336(11) Uani 1 1 d . . .
O3 O 0.2013(2) 0.1445(2) 0.4593(2) 0.0293(9) Uani 1 1 d . . .
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O5 O 0.4266(3) -0.1314(4) 0.6388(3) 0.0657(16) Uani 1 1 d D . .
C1 C 0.4086(4) 0.0131(3) 0.4100(4) 0.0346(14) Uani 1 1 d . . .
H1 H 0.4025 0.0608 0.3864 0.041 Uiso 1 1 calc R . .
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C6 C 0.6337(3) -0.2276(3) 0.4666(3) 0.0280(12) Uani 1 1 d . . .
H6 H 0.6892 -0.2241 0.4651 0.034 Uiso 1 1 calc R . .
C7 C 0.5976(3) -0.2996(3) 0.4797(3) 0.0248(11) Uani 1 1 d . . .
C8 C 0.5142(3) -0.3039(3) 0.4813(3) 0.0260(11) Uani 1 1 d . . .
H8 H 0.4895 -0.3516 0.4904 0.031 Uiso 1 1 calc R . .
C9 C 0.4684(3) -0.2386(3) 0.4697(3) 0.0269(12) Uani 1 1 d . . .
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C10 C 0.6476(3) -0.3705(3) 0.4916(3) 0.0274(12) Uani 1 1 d . . .
C11 C 0.2854(4) 0.0019(3) 0.6490(3) 0.0325(15) Uani 1 1 d . . .
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C15 C 0.2244(4) 0.2515(3) 0.7183(3) 0.0299(13) Uani 1 1 d . . .
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C16 C 0.2147(4) 0.3126(3) 0.7674(3) 0.0320(14) Uani 1 1 d . . .
H16 H 0.2084 0.3632 0.7498 0.038 Uiso 1 1 calc R . .
C17 C 0.2140(3) 0.3003(3) 0.8410(3) 0.0261(11) Uani 1 1 d . . .
C18 C 0.2229(3) 0.2240(3) 0.8675(3) 0.0264(12) Uani 1 1 d . . .
H18 H 0.2234 0.2154 0.9173 0.032 Uiso 1 1 calc R . .
C19 C 0.2309(3) 0.1614(3) 0.8206(3) 0.0278(12) Uani 1 1 d . . .
H19 H 0.2356 0.1107 0.8384 0.033 Uiso 1 1 calc R . .
C20 C 0.2072(3) 0.1310(3) 0.3916(3) 0.0262(11) Uani 1 1 d . . .
C21 C 0.5552(9) -0.2501(10) 0.7166(16) 0.280(19) Uani 1 1 d . . .
H21A H 0.6033 -0.2448 0.7456 0.336 Uiso 1 1 calc R . .
H21B H 0.5716 -0.2582 0.6667 0.336 Uiso 1 1 calc R . .
C22 C 0.5086(11) -0.3234(10) 0.7425(17) 0.251(17) Uani 1 1 d . . .
H22A H 0.5410 -0.3692 0.7356 0.376 Uiso 1 1 calc R . .
H22B H 0.4601 -0.3284 0.7150 0.376 Uiso 1 1 calc R . .
H22C H 0.4959 -0.3180 0.7931 0.376 Uiso 1 1 calc R . .
C23 C 0.5130(13) -0.1390(8) 0.7852(7) 0.177(10) Uani 1 1 d D . .
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H23B H 0.4647 -0.1076 0.7878 0.213 Uiso 1 1 calc R . .
C24 C 0.5847(10) -0.0857(7) 0.7945(7) 0.142(7) Uani 1 1 d D . .
H24A H 0.5802 -0.0579 0.8396 0.213 Uiso 1 1 calc R . .
H24B H 0.5866 -0.0490 0.7551 0.213 Uiso 1 1 calc R . .
H24C H 0.6327 -0.1165 0.7948 0.213 Uiso 1 1 calc R . .
C25 C 0.4744(8) -0.1694(10) 0.6667(9) 0.191(11) Uani 1 1 d D . .
H25 H 0.4901 -0.2072 0.6332 0.230 Uiso 1 1 calc R . .
OW1 O 0.4664(7) -0.4644(8) 0.5898(8) 0.180(5) Uani 1 1 d D . .

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N2 0.020(2) 0.022(2) 0.033(2) 0.0055(18) 0.0025(19) 0.0031(17)
N3 0.034(3) 0.021(2) 0.027(2) -0.0027(19) 0.000(2) 0.0019(19)
N4 0.033(3) 0.022(2) 0.026(2) -0.0028(19) -0.002(2) 0.0048(19)
N5 0.034(3) 0.091(6) 0.049(3) 0.001(4) -0.006(3) 0.013(3)
O1 0.038(3) 0.025(2) 0.056(3) 0.0138(19) 0.006(2) 0.0045(19)
O2 0.023(2) 0.023(2) 0.055(3) -0.0088(18) -0.0036(18) 0.0028(15)
O3 0.034(2) 0.023(2) 0.031(2) 0.0015(16) 0.0022(18) -0.0020(17)
O4 0.045(2) 0.0156(19) 0.030(2) -0.0009(16) 0.0018(18) -0.0013(16)
O5 0.060(4) 0.088(4) 0.049(3) 0.028(3) 0.008(3) 0.031(3)
C1 0.034(3) 0.030(3) 0.039(3) 0.011(3) 0.011(3) 0.004(2)
C2 0.030(3) 0.032(3) 0.052(4) 0.015(3) 0.013(3) 0.009(3)
C3 0.026(3) 0.017(3) 0.028(3) -0.0011(19) 0.000(2) -0.003(2)
C4 0.026(3) 0.021(3) 0.028(3) 0.001(2) -0.001(2) 0.001(2)
C5 0.022(3) 0.023(3) 0.041(3) 0.001(2) 0.001(2) -0.003(2)
C6 0.021(3) 0.024(3) 0.039(3) -0.005(2) 0.001(2) -0.001(2)
C7 0.022(3) 0.024(3) 0.027(3) 0.000(2) 0.001(2) 0.003(2)
C8 0.022(3) 0.021(3) 0.035(3) 0.003(2) -0.002(2) -0.004(2)
C9 0.022(3) 0.021(3) 0.038(3) 0.002(2) -0.002(2) -0.002(2)
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C13 0.032(3) 0.019(3) 0.025(3) 0.001(2) -0.002(2) 0.000(2)
C14 0.032(3) 0.017(3) 0.029(3) -0.004(2) -0.003(2) 0.000(2)
C15 0.048(4) 0.018(3) 0.023(3) -0.001(2) -0.002(2) -0.001(2)
C16 0.049(4) 0.017(3) 0.030(3) -0.001(2) -0.001(3) 0.006(2)
C17 0.027(3) 0.022(3) 0.030(3) 0.002(2) -0.003(2) -0.002(2)
C18 0.028(3) 0.024(3) 0.027(3) -0.002(2) 0.000(2) -0.001(2)
C19 0.032(3) 0.020(3) 0.031(3) 0.003(2) -0.001(2) 0.000(2)
C20 0.023(3) 0.023(3) 0.032(3) 0.004(2) 0.000(2) -0.002(2)
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C23 0.38(3) 0.086(9) 0.063(7) -0.013(7) 0.041(12) -0.090(14)
C24 0.228(18) 0.094(9) 0.105(9) -0.011(7) -0.099(11) -0.029(10)
C25 0.126(11) 0.258(19) 0.190(15) 0.196(15) -0.107(11) -0.135(13)
OW1 0.162(11) 0.205(12) 0.174(11) 0.008(11) 0.022(10) -0.005(11)

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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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C10 Cd1 N1 C1 149.6(6) 3_446 . . . ?
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_diffrn_detector_area_resol_mean  ?
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_diffrn_reflns_limit_h_min        -17
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_diffrn_reflns_limit_k_max        22
_diffrn_reflns_limit_l_min        -21
_diffrn_reflns_limit_l_max        21
_diffrn_reflns_theta_min          2.10
_diffrn_reflns_theta_max          26.50
_reflns_number_total              4988
_reflns_number_gt                 3769
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'SMART 5.628 (Bruker, 2003)'
_computing_cell_refinement        'SAINT 6.45 ( Bruker, 2003)'
_computing_data_reduction         'SAINT 6.45 ( Bruker, 2003)'
_computing_structure_solution     SIR-97
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
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_computing_molecular_graphics     'DIAMOND 2.1e'
_computing_publication_material   ?

_refine_special_details
;
 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.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0646P)^2^+10.5719P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     refU
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          4988
_refine_ls_number_parameters      344
_refine_ls_number_restraints      12
_refine_ls_R_factor_all           0.0662
_refine_ls_R_factor_gt            0.0452
_refine_ls_wR_factor_ref          0.1294
_refine_ls_wR_factor_gt           0.1110
_refine_ls_goodness_of_fit_ref    1.078
_refine_ls_restrained_S_all       1.095
_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

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Cd1 Cd 0.680403(19) 0.014181(17) 0.041169(17) 0.01327(12) Uani 1 1 d . . .
O1 O 0.67703(19) -0.12632(17) 0.08961(18) 0.0188(7) Uani 1 1 d . . .
O2 O 0.59259(19) -0.08200(16) -0.00180(17) 0.0184(7) Uani 1 1 d . . .
O3 O 0.7809(2) 0.35707(17) 0.51716(18) 0.0200(7) Uani 1 1 d . . .
O4 O 0.8560(2) 0.41272(16) 0.42556(18) 0.0192(7) Uani 1 1 d . . .
O5 O 1.0000 0.0583(3) 0.2500 0.079(3) Uani 1 2 d SD . .
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N1 N 0.7280(2) 0.0290(2) 0.1638(2) 0.0170(8) Uani 1 1 d . . .
N2 N 0.7501(2) 0.0964(2) 0.26792(19) 0.0169(8) Uani 1 1 d . . .
N3 N 0.4228(2) -0.4097(2) 0.0378(2) 0.0164(8) Uani 1 1 d . . .
N4 N 0.3104(2) -0.4817(2) 0.0137(2) 0.0173(8) Uani 1 1 d . . .
N5 N 1.0000 -0.0713(4) 0.2500 0.062(3) Uani 1 2 d SD . .
C1 C 0.6982(3) -0.0121(3) 0.2268(3) 0.0184(9) Uani 1 1 d . . .
H1 H 0.6735 -0.0600 0.2251 0.022 Uiso 1 1 calc R . .
C2 C 0.7115(3) 0.0297(3) 0.2909(2) 0.0215(10) Uani 1 1 d . . .
H2 H 0.6972 0.0161 0.3405 0.026 Uiso 1 1 calc R . .
C3 C 0.7574(3) 0.0935(2) 0.1909(2) 0.0176(9) Uani 1 1 d . . .
H3 H 0.7802 0.1322 0.1611 0.021 Uiso 1 1 calc R . .
C4 C 0.7677(3) 0.1612(2) 0.3141(2) 0.0175(9) Uani 1 1 d . . .
C5 C 0.8411(3) 0.2036(2) 0.3010(2) 0.0191(9) Uani 1 1 d . . .
H5 H 0.8802 0.1886 0.2638 0.023 Uiso 1 1 calc R . .
C6 C 0.8562(3) 0.2689(2) 0.3435(3) 0.0192(9) Uani 1 1 d . . .
H6 H 0.9037 0.2991 0.3330 0.023 Uiso 1 1 calc R . .
C7 C 0.7996(3) 0.2885(2) 0.4018(2) 0.0174(9) Uani 1 1 d . . .
C8 C 0.7273(3) 0.2443(3) 0.4146(3) 0.0232(10) Uani 1 1 d . . .
H8 H 0.6896 0.2573 0.4537 0.028 Uiso 1 1 calc R . .
C9 C 0.7099(3) 0.1813(3) 0.3705(3) 0.0235(10) Uani 1 1 d . . .
H9 H 0.6603 0.1529 0.3787 0.028 Uiso 1 1 calc R . .
C10 C 0.8142(3) 0.3575(3) 0.4510(2) 0.0154(9) Uani 1 1 d . . .
C11 C 0.6148(3) -0.1340(2) 0.0446(2) 0.0155(9) Uani 1 1 d . . .
C12 C 0.5658(3) -0.2075(3) 0.0426(2) 0.0167(9) Uani 1 1 d . . .
C13 C 0.5739(3) -0.2591(3) 0.1014(3) 0.0204(10) Uani 1 1 d . . .
H13 H 0.6095 -0.2479 0.1426 0.024 Uiso 1 1 calc R . .
C14 C 0.5295(3) -0.3275(3) 0.1001(3) 0.0213(10) Uani 1 1 d . . .
H14 H 0.5356 -0.3622 0.1396 0.026 Uiso 1 1 calc R . .
C15 C 0.4757(3) -0.3431(2) 0.0384(3) 0.0178(9) Uani 1 1 d . . .
C16 C 0.4693(3) -0.2927(2) -0.0221(3) 0.0195(10) Uani 1 1 d . . .
H16 H 0.4353 -0.3043 -0.0642 0.023 Uiso 1 1 calc R . .
C17 C 0.5139(3) -0.2250(3) -0.0194(3) 0.0200(9) Uani 1 1 d . . .
H17 H 0.5091 -0.1908 -0.0595 0.024 Uiso 1 1 calc R . .
C18 C 0.4384(3) -0.4790(3) 0.0720(3) 0.0263(11) Uani 1 1 d . . .
H18 H 0.4868 -0.4930 0.0998 0.032 Uiso 1 1 calc R . .
C19 C 0.3690(3) -0.5222(3) 0.0567(3) 0.0258(11) Uani 1 1 d . . .
H19 H 0.3616 -0.5720 0.0727 0.031 Uiso 1 1 calc R . .
C20 C 0.3452(3) -0.4146(3) 0.0036(3) 0.0192(9) Uani 1 1 d . . .
H20 H 0.3196 -0.3755 -0.0237 0.023 Uiso 1 1 calc R . .
C21 C 0.9483(7) -0.0051(8) 0.2492(6) 0.194(10) Uani 1 1 d D . .
C23 C 0.9332(9) -0.1267(11) 0.2541(9) 0.253(13) Uani 1 1 d D . .
OW1 O 0.5488(2) 0.05472(18) 0.09507(19) 0.0206(7) Uani 1 1 d D . .
OW2 O 0.7979(2) -0.2395(2) 0.1255(2) 0.0250(7) Uani 1 1 d D . .
OW3 O 0.4968(2) -0.0716(2) 0.1723(2) 0.0281(8) Uiso 1 1 d D . .
OW4 O 0.5651(3) 0.1750(2) 0.1962(2) 0.0349(9) Uiso 1 1 d D . .
H1W1 H 0.505(3) 0.055(3) 0.070(3) 0.045(19) Uiso 1 1 d D . .
H2W1 H 0.554(10) 0.076(8) 0.136(4) 0.03(7) Uiso 1 1 d D . .
H2W2 H 0.756(3) -0.214(3) 0.124(4) 0.05(2) Uiso 1 1 d D . .
H1W3 H 0.4477(17) -0.079(3) 0.158(3) 0.030(15) Uiso 1 1 d D . .
H2W3 H 0.516(6) -0.031(3) 0.159(5) 0.12(3) Uiso 1 1 d D . .
H1W4 H 0.603(4) 0.207(4) 0.189(5) 0.10(3) Uiso 1 1 d D . .
H4W4 H 0.524(3) 0.193(3) 0.176(3) 0.042(17) Uiso 1 1 d D . .

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O1 0.0194(17) 0.0152(16) 0.0219(16) -0.0032(12) -0.0017(13) -0.0019(12)
O2 0.0194(17) 0.0131(15) 0.0226(17) 0.0000(12) -0.0007(13) -0.0006(12)
O3 0.0245(18) 0.0148(16) 0.0205(16) -0.0026(12) 0.0032(13) -0.0009(13)
O4 0.0213(17) 0.0141(16) 0.0222(16) -0.0005(13) 0.0012(13) -0.0032(13)
O5 0.181(11) 0.020(3) 0.036(4) 0.000 0.037(5) 0.000
N1 0.022(2) 0.0160(19) 0.0131(18) 0.0018(14) -0.0024(15) -0.0015(15)
N2 0.024(2) 0.0152(19) 0.0114(17) -0.0003(14) -0.0017(15) -0.0037(15)
N3 0.0178(19) 0.0107(18) 0.0206(19) 0.0014(14) -0.0016(15) -0.0015(14)
N4 0.020(2) 0.014(2) 0.0179(19) -0.0002(15) -0.0008(15) -0.0003(14)
N5 0.106(7) 0.016(3) 0.063(5) 0.000 -0.053(5) 0.000
C1 0.022(2) 0.014(2) 0.019(2) 0.0034(17) -0.0011(18) -0.0055(17)
C2 0.031(3) 0.020(2) 0.014(2) 0.0043(17) 0.0009(19) -0.0079(19)
C3 0.019(2) 0.017(2) 0.017(2) 0.0027(17) 0.0007(18) -0.0031(17)
C4 0.022(2) 0.013(2) 0.018(2) -0.0003(17) -0.0037(18) -0.0029(17)
C5 0.020(2) 0.018(2) 0.018(2) -0.0008(18) 0.0011(18) 0.0012(18)
C6 0.022(2) 0.017(2) 0.019(2) -0.0011(17) 0.0009(18) -0.0042(18)
C7 0.020(2) 0.014(2) 0.018(2) 0.0000(17) -0.0036(18) 0.0007(17)
C8 0.024(3) 0.024(3) 0.021(2) -0.0003(19) 0.0070(19) -0.0069(19)
C9 0.021(2) 0.026(3) 0.023(2) -0.003(2) 0.0007(19) -0.008(2)
C10 0.016(2) 0.016(2) 0.015(2) -0.0011(16) -0.0035(17) 0.0050(16)
C11 0.014(2) 0.014(2) 0.019(2) -0.0045(17) 0.0046(17) 0.0005(16)
C12 0.014(2) 0.017(2) 0.019(2) -0.0002(17) 0.0021(17) -0.0001(17)
C13 0.022(2) 0.018(2) 0.021(2) 0.0004(18) -0.0031(19) -0.0036(18)
C14 0.020(2) 0.021(2) 0.023(2) 0.0038(19) -0.0010(19) 0.0000(18)
C15 0.015(2) 0.013(2) 0.026(2) -0.0031(17) 0.0017(18) 0.0001(17)
C16 0.019(2) 0.017(2) 0.023(2) -0.0030(18) -0.0044(18) -0.0022(18)
C17 0.020(2) 0.015(2) 0.025(2) 0.0005(18) 0.0020(18) -0.0014(18)
C18 0.027(3) 0.019(3) 0.032(3) 0.012(2) -0.010(2) -0.0044(19)
C19 0.024(3) 0.020(3) 0.033(3) 0.009(2) -0.009(2) -0.0033(19)
C20 0.017(2) 0.018(2) 0.023(2) 0.0017(18) -0.0018(18) -0.0005(18)
C21 0.120(11) 0.40(3) 0.060(7) 0.106(12) 0.033(7) 0.148(15)
C23 0.106(11) 0.46(3) 0.197(16) -0.23(2) 0.049(11) -0.113(16)
OW1 0.0198(18) 0.0216(17) 0.0204(17) -0.0005(13) -0.0009(14) 0.0004(14)
OW2 0.0231(19) 0.0224(19) 0.0295(18) 0.0028(15) 0.0002(15) 0.0040(14)

_geom_special_details
;
 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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Cd1 N1 2.287(4) . ?
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Cd1 O2 2.306(3) . ?
Cd1 N4 2.310(4) 3_545 ?
Cd1 OW1 2.364(3) . ?
Cd1 O3 2.390(3) 2_654 ?
Cd1 O4 2.468(3) 2_654 ?
Cd1 O1 2.624(3) . ?
O1 C11 1.255(5) . ?
O2 C11 1.275(5) . ?
O3 C10 1.269(5) . ?
O3 Cd1 2.390(3) 2_655 ?
O4 C10 1.254(5) . ?
O4 Cd1 2.468(3) 2_655 ?
O5 C21 1.378(14) . ?
O5 C21 1.378(14) 4_755 ?
N1 C3 1.317(6) . ?
N1 C1 1.400(6) . ?
N2 C3 1.355(5) . ?
N2 C2 1.382(6) . ?
N2 C4 1.428(5) . ?
N3 C20 1.350(6) . ?
N3 C18 1.385(6) . ?
N3 C15 1.435(6) . ?
N4 C20 1.314(6) . ?
N4 C19 1.381(6) . ?
N4 Cd1 2.310(4) 3_445 ?
N5 C21 1.419(11) 4_755 ?
N5 C21 1.419(11) . ?
N5 C23 1.430(12) 4_755 ?
N5 C23 1.430(12) . ?
C1 C2 1.359(6) . ?
C4 C9 1.382(6) . ?
C4 C5 1.384(6) . ?
C5 C6 1.392(6) . ?
C6 C7 1.392(6) . ?
C7 C8 1.387(6) . ?
C7 C10 1.510(6) . ?
C8 C9 1.381(7) . ?
C11 C12 1.505(6) . ?
C12 C13 1.382(6) . ?
C12 C17 1.387(6) . ?
C13 C14 1.392(6) . ?
C14 C15 1.393(6) . ?
C15 C16 1.389(6) . ?
C16 C17 1.383(6) . ?
C18 C19 1.347(7) . ?
C21 C21 1.61(2) 4_755 ?

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N1 Cd1 N4 97.84(14) . 3_545 ?
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N1 Cd1 OW1 82.54(13) . . ?
O2 Cd1 OW1 80.88(11) . . ?
N4 Cd1 OW1 176.70(12) 3_545 . ?
N1 Cd1 O3 88.56(12) . 2_654 ?
O2 Cd1 O3 142.45(11) . 2_654 ?
N4 Cd1 O3 86.74(12) 3_545 2_654 ?
OW1 Cd1 O3 89.99(11) . 2_654 ?
N1 Cd1 O4 141.73(11) . 2_654 ?
O2 Cd1 O4 88.97(10) . 2_654 ?
N4 Cd1 O4 89.36(12) 3_545 2_654 ?
OW1 Cd1 O4 88.34(11) . 2_654 ?
O3 Cd1 O4 54.21(10) 2_654 2_654 ?
N1 Cd1 O1 79.10(11) . . ?
O2 Cd1 O1 52.89(10) . . ?
N4 Cd1 O1 85.24(11) 3_545 . ?
OW1 Cd1 O1 98.05(10) . . ?
O3 Cd1 O1 164.21(10) 2_654 . ?
O4 Cd1 O1 139.11(10) 2_654 . ?
C11 O1 Cd1 85.1(2) . . ?
C11 O2 Cd1 99.4(3) . . ?
C10 O3 Cd1 93.0(3) . 2_655 ?
C10 O4 Cd1 89.8(2) . 2_655 ?
C21 O5 C21 71.3(9) . 4_755 ?
C3 N1 C1 106.2(4) . . ?
C3 N1 Cd1 123.4(3) . . ?
C1 N1 Cd1 125.1(3) . . ?
C3 N2 C2 107.1(4) . . ?
C3 N2 C4 125.3(4) . . ?
C2 N2 C4 127.0(4) . . ?
C20 N3 C18 106.9(4) . . ?
C20 N3 C15 124.6(4) . . ?
C18 N3 C15 128.4(4) . . ?
C20 N4 C19 105.6(4) . . ?
C20 N4 Cd1 121.9(3) . 3_445 ?
C19 N4 Cd1 132.4(3) . 3_445 ?
C21 N5 C21 69.0(12) 4_755 . ?
C21 N5 C23 98.9(9) 4_755 4_755 ?
C21 N5 C23 167.3(10) . 4_755 ?
C21 N5 C23 167.3(10) 4_755 . ?
C21 N5 C23 98.9(9) . . ?
C23 N5 C23 93.5(17) 4_755 . ?
C2 C1 N1 108.6(4) . . ?
C1 C2 N2 106.8(4) . . ?
N1 C3 N2 111.3(4) . . ?
C9 C4 C5 120.9(4) . . ?
C9 C4 N2 119.2(4) . . ?
C5 C4 N2 119.9(4) . . ?
C4 C5 C6 120.0(4) . . ?
C7 C6 C5 119.5(4) . . ?
C8 C7 C6 119.3(4) . . ?
C8 C7 C10 119.0(4) . . ?
C6 C7 C10 121.7(4) . . ?
C9 C8 C7 121.5(4) . . ?
C8 C9 C4 118.7(4) . . ?
O4 C10 O3 122.8(4) . . ?
O4 C10 C7 120.1(4) . . ?
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O3 C10 C7 117.1(4) . . ?
O1 C11 O2 122.1(4) . . ?
O1 C11 C12 119.9(4) . . ?
O2 C11 C12 118.0(4) . . ?
C13 C12 C17 119.3(4) . . ?
C13 C12 C11 120.4(4) . . ?
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C12 C13 C14 121.0(4) . . ?
C13 C14 C15 118.9(4) . . ?
C16 C15 C14 120.5(4) . . ?
C16 C15 N3 118.6(4) . . ?
C14 C15 N3 120.8(4) . . ?
C17 C16 C15 119.5(4) . . ?
C16 C17 C12 120.8(4) . . ?
C19 C18 N3 105.9(4) . . ?
C18 C19 N4 110.1(4) . . ?
N4 C20 N3 111.5(4) . . ?
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O5 C21 C21 54.4(4) . 4_755 ?
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OW1 Cd1 O1 C11 67.9(2) . . . . ?
O3 Cd1 O1 C11 -172.1(4) 2_654 . . . ?
O4 Cd1 O1 C11 -28.9(3) 2_654 . . . ?
N1 Cd1 O2 C11 -29.4(3) . . . . ?
N4 Cd1 O2 C11 79.1(3) 3_545 . . . ?
OW1 Cd1 O2 C11 -103.3(3) . . . . ?
O3 Cd1 O2 C11 178.8(2) 2_654 . . . ?
O4 Cd1 O2 C11 168.2(3) 2_654 . . . ?
O1 Cd1 O2 C11 4.1(2) . . . . ?
O2 Cd1 N1 C3 -160.7(3) . . . . ?
N4 Cd1 N1 C3 89.1(4) 3_545 . . . ?
OW1 Cd1 N1 C3 -87.6(4) . . . . ?
O3 Cd1 N1 C3 2.6(4) 2_654 . . . ?
O4 Cd1 N1 C3 -9.9(5) 2_654 . . . ?
O1 Cd1 N1 C3 172.7(4) . . . . ?
O2 Cd1 N1 C1 -10.2(4) . . . . ?
N4 Cd1 N1 C1 -120.4(4) 3_545 . . . ?
OW1 Cd1 N1 C1 62.9(4) . . . . ?
O3 Cd1 N1 C1 153.1(4) 2_654 . . . ?
O4 Cd1 N1 C1 140.6(3) 2_654 . . . ?
O1 Cd1 N1 C1 -36.8(3) . . . . ?
C3 N1 C1 C2 -0.4(5) . . . . ?
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Cd1 N1 C1 C2 -155.0(3) . . . . ?
N1 C1 C2 N2 -0.6(5) . . . . ?
C3 N2 C2 C1 1.3(5) . . . . ?
C4 N2 C2 C1 172.7(4) . . . . ?
C1 N1 C3 N2 1.2(5) . . . . ?
Cd1 N1 C3 N2 156.4(3) . . . . ?
C2 N2 C3 N1 -1.6(5) . . . . ?
C4 N2 C3 N1 -173.2(4) . . . . ?
C3 N2 C4 C9 133.9(5) . . . . ?
C2 N2 C4 C9 -36.0(7) . . . . ?
C3 N2 C4 C5 -44.9(6) . . . . ?
C2 N2 C4 C5 145.2(5) . . . . ?
C9 C4 C5 C6 -1.9(7) . . . . ?
N2 C4 C5 C6 176.9(4) . . . . ?
C4 C5 C6 C7 3.6(7) . . . . ?
C5 C6 C7 C8 -2.5(7) . . . . ?
C5 C6 C7 C10 178.4(4) . . . . ?
C6 C7 C8 C9 -0.2(7) . . . . ?
C10 C7 C8 C9 178.9(4) . . . . ?
C7 C8 C9 C4 1.9(7) . . . . ?
C5 C4 C9 C8 -0.8(7) . . . . ?
N2 C4 C9 C8 -179.7(4) . . . . ?
Cd1 O4 C10 O3 -5.2(4) 2_655 . . . ?
Cd1 O4 C10 C7 173.2(3) 2_655 . . . ?
Cd1 O3 C10 O4 5.4(4) 2_655 . . . ?
Cd1 O3 C10 C7 -173.1(3) 2_655 . . . ?
C8 C7 C10 O4 -152.7(4) . . . . ?
C6 C7 C10 O4 26.4(6) . . . . ?
C8 C7 C10 O3 25.8(6) . . . . ?
C6 C7 C10 O3 -155.1(4) . . . . ?
Cd1 O1 C11 O2 7.1(4) . . . . ?
Cd1 O1 C11 C12 -175.0(4) . . . . ?
Cd1 O2 C11 O1 -8.1(4) . . . . ?
Cd1 O2 C11 C12 173.9(3) . . . . ?
O1 C11 C12 C13 16.1(6) . . . . ?
O2 C11 C12 C13 -165.8(4) . . . . ?
O1 C11 C12 C17 -162.1(4) . . . . ?
O2 C11 C12 C17 16.0(6) . . . . ?
C17 C12 C13 C14 -1.3(7) . . . . ?
C11 C12 C13 C14 -179.5(4) . . . . ?
C12 C13 C14 C15 -0.6(7) . . . . ?
C13 C14 C15 C16 2.7(7) . . . . ?
C13 C14 C15 N3 -174.4(4) . . . . ?
C20 N3 C15 C16 -28.7(6) . . . . ?
C18 N3 C15 C16 153.0(5) . . . . ?
C20 N3 C15 C14 148.4(4) . . . . ?
C18 N3 C15 C14 -29.9(7) . . . . ?
C14 C15 C16 C17 -2.9(7) . . . . ?
N3 C15 C16 C17 174.3(4) . . . . ?
C15 C16 C17 C12 1.0(7) . . . . ?
C13 C12 C17 C16 1.1(7) . . . . ?
C11 C12 C17 C16 179.3(4) . . . . ?
C20 N3 C18 C19 -0.1(6) . . . . ?
C15 N3 C18 C19 178.4(4) . . . . ?
N3 C18 C19 N4 0.1(6) . . . . ?
C20 N4 C19 C18 0.0(6) . . . . ?
Cd1 N4 C19 C18 176.4(3) 3_445 . . . ?
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C19 N4 C20 N3 -0.1(5) . . . . ?
Cd1 N4 C20 N3 -176.9(3) 3_445 . . . ?
C18 N3 C20 N4 0.2(5) . . . . ?
C15 N3 C20 N4 -178.4(4) . . . . ?
C21 O5 C21 N5 0.0 4_755 . . . ?
C21 N5 C21 O5 0.0 4_755 . . . ?
C23 N5 C21 O5 -17(5) 4_755 . . . ?
C23 N5 C21 O5 176.4(9) . . . . ?
C23 N5 C21 C21 -17(5) 4_755 . . 4_755 ?
C23 N5 C21 C21 176.4(9) . . . 4_755 ?

_diffrn_measured_fraction_theta_max    0.999
_diffrn_reflns_theta_full              26.50
_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    1.338
_refine_diff_density_min   -1.205
_refine_diff_density_rms    0.229

#===END
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