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 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-
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N5 N 0.2782(2) -0.41888(15) 0.68028(18) 0.0372(7) Uani 1 1 d . . .
C1 C 0.4012(3) -0.5666(2) 0.5755(3) 0.0439(10) Uani 1 1 d . . .
C2 C 0.4762(3) -0.5535(2) 0.6723(3) 0.0642(13) Uani 0.813(4) 1 d PD B 3
H2A H 0.5129 -0.5050 0.6554 0.077 Uiso 0.813(4) 1 calc PRD B 3
C3 C 0.5611(3) -0.6056(3) 0.6903(3) 0.0579(15) Uani 0.813(4) 1 d PD B 3
H3A H 0.5367 -0.6581 0.7056 0.070 Uiso 0.813(4) 1 calc PR B 3
C4 C 0.6603(3) -0.5826(3) 0.7544(3) 0.0727(14) Uani 0.813(4) 1 d P B 3
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C5 C 0.6645(2) -0.6020(2) 0.6386(3) 0.0685(14) Uani 0.813(4) 1 d P B 3
H5A H 0.6763 -0.5604 0.5869 0.082 Uiso 0.813(4) 1 calc PR B 3
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C2' C 0.4762(3) -0.5535(2) 0.6723(3) 0.0642(13) Uani 0.19 1 d PD B 4
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H2′A H 0.4888 -0.6078 0.6897 0.077 Uiso 0.187(4) 1 calc PRD B 4
C3′ C 0.5795 -0.5350 0.6596 0.099 Uani 0.19 1 d PD B 4
H3′A H 0.5981 -0.4822 0.6390 0.119 Uiso 0.187(4) 1 calc PR B 4
C4′ C 0.6603(3) -0.5826(3) 0.7544(3) 0.0727(14) Uani 0.19 1 d P B 4
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H4′B H 0.6257 -0.6189 0.8033 0.087 Uiso 0.187(4) 1 calc PR B 4
C5′ C 0.6645(2) -0.6020(2) 0.6386(3) 0.0685(14) Uani 0.19 1 d P B 4
H5′A H 0.6350 -0.6516 0.6167 0.082 Uiso 0.187(4) 1 calc PR B 4
H5′B H 0.7302 -0.5881 0.6007 0.082 Uiso 0.187(4) 1 calc PR B 4
C6 C 0.2699(3) -0.6919(2) 0.7233(3) 0.0522(10) Uani 1 1 d . B .
H6 H 0.2898 -0.6873 0.6499 0.063 Uiso 1 1 calc R . .
C7 C 0.2685(3) -0.7630(2) 0.7689(4) 0.0686(12) Uani 1 1 d . . .
H7 H 0.2895 -0.8058 0.7285 0.082 Uiso 1 1 calc R B .
C8 C 0.2360(3) -0.7705(3) 0.8742(4) 0.0738(13) Uani 1 1 d . B .
H8 H 0.2338 -0.8187 0.9076 0.089 Uiso 1 1 calc R . .
C9 C 0.2068(3) -0.7068(3) 0.9302(3) 0.0584(11) Uani 1 1 d . . .
H9 H 0.1823 -0.7110 1.0021 0.070 Uiso 1 1 calc R B .
C10 C 0.2132(2) -0.6363(2) 0.8808(3) 0.0433(10) Uani 1 1 d . B .
C11 C 0.1904(2) -0.5647(2) 0.9331(3) 0.0425(10) Uani 1 1 d . B .
C12 C 0.1447(3) -0.5575(3) 1.0333(3) 0.0632(13) Uani 1 1 d . . .
H12 H 0.1284 -0.6008 1.0750 0.076 Uiso 1 1 calc R B .
C13 C 0.1230(3) -0.4860(3) 1.0716(3) 0.0697(14) Uani 1 1 d . B .
H13 H 0.0892 -0.4802 1.1391 0.084 Uiso 1 1 calc R . .
C14 C 0.1501(3) -0.4227(3) 1.0126(3) 0.0600(12) Uani 1 1 d . . .
H14 H 0.1366 -0.3735 1.0393 0.072 Uiso 1 1 calc R B .
C15 C 0.1973(2) -0.4332(2) 0.9136(3) 0.0453(10) Uani 1 1 d . B .
H15 H 0.2164 -0.3903 0.8723 0.054 Uiso 1 1 calc R . .
C16 C 0.0371(2) -0.5603(2) 0.6829(2) 0.0376(9) Uani 1 1 d . B .
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C17 C -0.0655(2) -0.5442(2) 0.6479(2) 0.0424(10) Uani 1 1 d . . .
H17 H -0.1200 -0.5811 0.6526 0.051 Uiso 1 1 calc R B .
C18 C -0.0882(2) -0.4734(2) 0.6057(2) 0.0431(9) Uani 1 1 d . B .
H18 H -0.1585 -0.4614 0.5815 0.052 Uiso 1 1 calc R . .
C19 C -0.0078(3) -0.4206(2) 0.5992(2) 0.0397(9) Uani 1 1 d . . .
H19 H -0.0222 -0.3720 0.5703 0.048 Uiso 1 1 calc R B .
C20 C 0.0951(3) -0.4397(2) 0.6360(2) 0.0334(8) Uani 1 1 d . B .
C21 C 0.1879(2) -0.3891(2) 0.6333(2) 0.0333(8) Uani 1 1 d . B .
C22 C 0.1876(3) -0.3191(2) 0.5850(2) 0.0390(9) Uani 1 1 d . . .
H22 H 0.1239 -0.2997 0.5527 0.047 Uiso 1 1 calc R B .
C23 C 0.2798(3) -0.2774(2) 0.5838(2) 0.0455(10) Uani 1 1 d . B .
H23 H 0.2807 -0.2294 0.5500 0.055 Uiso 1 1 calc R . .
C24 C 0.3716(3) -0.3065(2) 0.6328(3) 0.0481(10) Uani 1 1 d . . .
H24 H 0.4361 -0.2785 0.6335 0.058 Uiso 1 1 calc R B .
C25 C 0.3673(3) -0.3767(2) 0.6805(3) 0.0455(10) Uani 1 1 d . B .
H25 H 0.4300 -0.3962 0.7149 0.055 Uiso 1 1 calc R . .
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O2 O 0.43477(17) -0.58864(14) 0.48839(18) 0.0603(7) Uani 1 1 d . B .
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O14 O 0.14464(17) -0.23985(13) 0.35390(17) 0.0541(7) Uani 1 1 d . . .
Cl2 Cl 0.51762(8) -0.14449(7) 0.44938(7) 0.0517(3) Uani 1 1 d . . .
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O22′ O 0.558(2) -0.0823(14) 0.4055(17) 0.183(9) Uani 0.49(2) 1 d P C 2
O23′ O 0.4059(9) -0.151(2) 0.4322(12) 0.148(10) Uani 0.49(2) 1 d P C 2
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O23’ 0.024(4) 0.32(3) 0.100(7) 0.071(13) -0.021(4) -0.026(10)
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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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C4 C5 1.474(5) . ?
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O21' Cl2 O22 84.4(14) . . ?
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 '-x, -y, -z'

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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O32 O 0.1708(3) -0.77885(14) 0.02448(15) 0.0588(7) Uani 1 1 d . . .
O33 O -0.0028(4) -0.65682(18) 0.76904(16) 0.0882(11) Uani 1 1 d . . .
O34 O 0.0748(2) -0.08360(18) -0.1388(2) 0.0796(10) Uani 1 1 d . . .
O41 O 0.7268(3) -1.11719(19) 0.58892(18) 0.0827(9) Uani 1 1 d . . .
O42 O 0.3440(2) -0.68651(18) -0.03003(18) 0.0669(7) Uani 1 1 d . . .
O43 O 0.0222(3) -0.56210(14) 0.64088(13) 0.0510(6) Uani 1 1 d . . .
O44 O 0.2408(3) -0.17554(15) -0.08889(16) 0.0625(7) Uani 1 1 d . . .
O50 O 0.2718(2) -1.05816(14) 0.47441(12) 0.0448(5) Uani 1 1 d . . .
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H501 H 0.3225 -1.1091 0.4991 0.067 Uiso 1 1 d R . .
H502 H 0.3172 -1.0127 0.4808 0.067 Uiso 1 1 d R . .
O51 O 0.3367(2) -1.21678(16) 0.55899(16) 0.0619(7) Uani 1 1 d . . .
H512 H 0.4109 -1.2230 0.5905 0.093 Uiso 1 1 d R . .
H511 H 0.2816 -1.2598 0.5809 0.093 Uiso 1 1 d R . .
O60 O 0.1296(2) -0.32956(15) -0.07353(17) 0.0618(7) Uani 1 1 d . . .
H601 H 0.0487 -0.3306 -0.0486 0.093 Uiso 1 1 d R . .
H602 H 0.1578 -0.2795 -0.0851 0.093 Uiso 1 1 d R . .
O61 O 0.26234(19) -0.48197(12) -0.05792(11) 0.0355(5) Uani 1 1 d . . .
H612 H 0.2121 -0.5199 -0.0352 0.053 Uiso 1 1 d R . .
H611 H 0.2194 -0.4401 -0.0582 0.053 Uiso 1 1 d R . .
O1 O 0.63180(18) -0.57885(11) 0.34618(10) 0.0284(4) Uani 1 1 d . . .
O1′ O 0.36428(18) -0.12869(11) 0.22803(10) 0.0279(4) Uani 1 1 d . . .
O2 O 0.8233(2) -0.64089(13) 0.37252(12) 0.0450(6) Uani 1 1 d . . .
O2′ O 0.5663(2) -0.18279(13) 0.23733(13) 0.0426(5) Uani 1 1 d . . .
N1 N 0.7191(2) -0.47426(13) 0.20882(12) 0.0249(5) Uani 1 1 d . B .
H1A H 0.7227 -0.4910 0.1636 0.030 Uiso 1 1 calc R . .
H1B H 0.7333 -0.4182 0.1930 0.030 Uiso 1 1 calc R . .
N1′ N 0.3726(2) -0.01580(13) 0.30049(13) 0.0260(5) Uani 1 1 d . A .
H1′1 H 0.3866 0.0403 0.2840 0.031 Uiso 1 1 calc R . .
H1′2 H 0.3391 -0.0302 0.3542 0.031 Uiso 1 1 calc R . .
N2 N 0.5201(2) -0.56551(13) 0.21172(12) 0.0254(5) Uani 1 1 d . . .
N2′ N 0.1535(2) -0.10122(14) 0.34244(13) 0.0287(5) Uani 1 1 d . . .
N3 N 0.4540(2) -0.41032(12) 0.19716(12) 0.0220(4) Uani 1 1 d . . .
N3′ N 0.1283(2) 0.05305(13) 0.26207(13) 0.0266(5) Uani 1 1 d . . .
N4 N 0.3829(2) -0.52097(13) 0.34840(12) 0.0268(5) Uani 1 1 d . . .
N4′ N 0.1347(2) -0.06941(13) 0.17992(12) 0.0243(5) Uani 1 1 d . . .
N5 N 0.5584(2) -0.41818(13) 0.33799(12) 0.0273(5) Uani 1 1 d . . .
N5′ N 0.3292(2) 0.02775(13) 0.13571(12) 0.0245(5) Uani 1 1 d . . .
C1′ C 0.4789(3) -0.13180(17) 0.24895(16) 0.0292(6) Uani 1 1 d . A .
C1 C 0.7588(3) -0.58597(17) 0.32958(16) 0.0312(6) Uani 1 1 d . B .
C2′ C 0.4993(3) -0.06420(19) 0.28767(19) 0.0359(7) Uani 1 1 d D . .
H2′ H 0.5616 -0.0302 0.2494 0.043 Uiso 0.845(8) 1 d PRD A 1
H20′ H 0.4628 -0.0972 0.3285 0.043 Uiso 0.155(8) 1 d PRD A 2
C3′ C 0.5565(4) -0.0982(2) 0.3624(2) 0.0325(10) Uani 0.845(8) 1 d PD A 1
H3′A H 0.5099 -0.1448 0.4041 0.039 Uiso 0.845(8) 1 calc PR A 1
C30′ C 0.604(3) -0.077(3) 0.335(2) 0.097(15) Uani 0.155(8) 1 d PD A 2
H30A H 0.5571 -0.1236 0.3769 0.117 Uiso 0.155(8) 1 calc PR A 2
C2 C 0.8238(3) -0.52210(18) 0.25525(16) 0.0314(7) Uani 0.977(5) 1 d PD . .
H2 H 0.8718 -0.4823 0.2719 0.038 Uiso 0.977(5) 1 d PRD B 3
H20 H 0.8207 -0.5495 0.2227 0.038 Uiso 0.023(5) 1 d PRD B 4
C3 C 0.9295(3) -0.5614(2) 0.20536(18) 0.0360(8) Uani 0.977(5) 1 d PD B 3
H3A H 0.9038 -0.6096 0.1906 0.043 Uiso 0.977(5) 1 calc PR B 3
C30 C 0.962(3) -0.509(5) 0.218(3) 0.01(2) Uani 0.023(5) 1 d PD B 4
H30B H 0.9895 -0.4611 0.2332 0.008 Uiso 0.023(5) 1 calc PR B 4
C4′ C 0.6150(4) -0.0376(2) 0.3940(2) 0.0585(12) Uani 0.845(8) 1 d P A 1
H4′A H 0.6166 0.0217 0.3617 0.070 Uiso 0.845(8) 1 calc PR A 1
H4′B H 0.6015 -0.0469 0.4527 0.070 Uiso 0.845(8) 1 calc PR A 1
C5′ C 0.7015(4) -0.1004(2) 0.3606(3) 0.0590(12) Uani 0.845(8) 1 d P A 1
H5′A H 0.7569 -0.0796 0.3078 0.071 Uiso 0.845(8) 1 calc PR A 1
H5′B H 0.7418 -0.1480 0.3987 0.071 Uiso 0.845(8) 1 calc PR A 1
C40′ C 0.6150(4) -0.0376(2) 0.3940(2) 0.0585(12) Uani 0.15 1 d P A 2
H40A H 0.5623 -0.0567 0.4479 0.070 Uiso 0.155(8) 1 calc PR A 2
H40B H 0.6394 0.0212 0.3764 0.070 Uiso 0.155(8) 1 calc PR A 2
C50′ C 0.7015(4) -0.1004(2) 0.3606(3) 0.0590(12) Uani 0.15 1 d P A 2
H50A H 0.7841 -0.0812 0.3251 0.071 Uiso 0.155(8) 1 calc PR A 2
H50B H 0.7078 -0.1583 0.3958 0.071 Uiso 0.155(8) 1 calc PR A 2
C4 C 1.0264(3) -0.5057(2) 0.1430(2) 0.0453(9) Uani 0.977(5) 1 d P B 3
H4A H 1.0561 -0.5192 0.0917 0.054 Uiso 0.977(5) 1 calc PR B 3
H4B H 1.0186 -0.4454 0.1388 0.054 Uiso 0.977(5) 1 calc PR B 3
C5 C 1.0686(3) -0.5647(2) 0.2165(2) 0.0457(9) Uani 0.977(5) 1 d P B 3
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H5A H 1.0877 -0.5408 0.2577 0.055 Uiso 0.977(5) 1 calc PR B 3
H5B H 1.1251 -0.6145 0.2107 0.055 Uiso 0.977(5) 1 calc PR B 3
C40 C 1.0264(3) -0.5057(2) 0.1430(2) 0.0453(9) Uani 0.02 1 d P B 4
H40C H 1.0801 -0.4575 0.1139 0.054 Uiso 0.023(5) 1 calc PR B 4
H40D H 0.9840 -0.5286 0.1091 0.054 Uiso 0.023(5) 1 calc PR B 4
C50 C 1.0686(3) -0.5647(2) 0.2165(2) 0.0457(9) Uani 0.02 1 d P B 4
H50C H 1.0525 -0.6245 0.2286 0.055 Uiso 0.023(5) 1 calc PR B 4
H50D H 1.1486 -0.5534 0.2334 0.055 Uiso 0.023(5) 1 calc PR B 4
C6′ C 0.1768(3) -0.18276(18) 0.37833(17) 0.0350(6) Uani 1 1 d . . .
H6′ H 0.2436 -0.2139 0.3532 0.042 Uiso 1 1 calc R . .
C6 C 0.5680(3) -0.64540(16) 0.22208(16) 0.0304(6) Uani 1 1 d . . .
H6 H 0.6168 -0.6706 0.2645 0.037 Uiso 1 1 calc R . .
C7′ C 0.1042(3) -0.2225(2) 0.45200(18) 0.0430(8) Uani 1 1 d . . .
H7′ H 0.1226 -0.2800 0.4772 0.052 Uiso 1 1 calc R . .
C7 C 0.5483(3) -0.69175(18) 0.17279(18) 0.0365(7) Uani 1 1 d . . .
H7 H 0.5839 -0.7476 0.1809 0.044 Uiso 1 1 calc R . .
C8′ C 0.0056(3) -0.1776(2) 0.48790(18) 0.0473(8) Uani 1 1 d . . .
H8′ H -0.0449 -0.2040 0.5378 0.057 Uiso 1 1 calc R . .
C8 C 0.4766(3) -0.65585(19) 0.11216(18) 0.0388(7) Uani 1 1 d . . .
H8 H 0.4613 -0.6867 0.0781 0.047 Uiso 1 1 calc R . .
C9′ C -0.0188(3) -0.0936(2) 0.45012(18) 0.0420(7) Uani 1 1 d . . .
H9′ H -0.0869 -0.0619 0.4737 0.050 Uiso 1 1 calc R . .
C9 C 0.4267(3) -0.57396(18) 0.10115(17) 0.0339(6) Uani 1 1 d . . .
H9 H 0.3761 -0.5484 0.0598 0.041 Uiso 1 1 calc R . .
C10′ C 0.0568(3) -0.05644(19) 0.37783(16) 0.0316(6) Uani 1 1 d . . .
C10 C 0.4515(2) -0.52964(16) 0.15119(15) 0.0253(5) Uani 1 1 d . . .
C11′ C 0.0433(3) 0.03221(18) 0.33212(16) 0.0319(6) Uani 1 1 d . . .
C11 C 0.4097(2) -0.44184(16) 0.14486(15) 0.0245(5) Uani 1 1 d . . .
C12′ C -0.0450(3) 0.0915(2) 0.35652(19) 0.0432(8) Uani 1 1 d . . .
H12′ H -0.1038 0.0762 0.4056 0.052 Uiso 1 1 calc R . .
C12 C 0.3319(3) -0.39283(17) 0.09092(16) 0.0314(6) Uani 1 1 d . . .
H12 H 0.3011 -0.4154 0.0549 0.038 Uiso 1 1 calc R . .
C13′ C -0.0458(3) 0.1733(2) 0.3082(2) 0.0472(8) Uani 1 1 d . . .
H13′ H -0.1047 0.2148 0.3240 0.057 Uiso 1 1 calc R . .
C13 C 0.2993(3) -0.31036(17) 0.08995(17) 0.0333(6) Uani 1 1 d . . .
H13 H 0.2447 -0.2762 0.0539 0.040 Uiso 1 1 calc R . .
C14′ C 0.0396(3) 0.19386(19) 0.2369(2) 0.0405(7) Uani 1 1 d . . .
H14′ H 0.0394 0.2496 0.2030 0.049 Uiso 1 1 calc R . .
C14 C 0.3469(3) -0.27834(16) 0.14179(16) 0.0290(6) Uani 1 1 d . . .
H14 H 0.3264 -0.2218 0.1413 0.035 Uiso 1 1 calc R . .
C15′ C 0.1254(3) 0.13284(17) 0.21517(17) 0.0317(6) Uani 1 1 d . . .
H15′ H 0.1840 0.1474 0.1660 0.038 Uiso 1 1 calc R . .
C15 C 0.4246(3) -0.32957(16) 0.19447(15) 0.0256(5) Uani 1 1 d . . .
H15 H 0.4582 -0.3073 0.2297 0.031 Uiso 1 1 calc R . .
C16′ C 0.0328(3) -0.11959(17) 0.20851(17) 0.0316(6) Uani 1 1 d . . .
H16′ H 0.0040 -0.1375 0.2646 0.038 Uiso 1 1 calc R . .
C16 C 0.2995(3) -0.57709(18) 0.34938(17) 0.0350(7) Uani 1 1 d . . .
H16 H 0.3161 -0.6046 0.3087 0.042 Uiso 1 1 calc R . .
C17′ C -0.0307(3) -0.14566(18) 0.15869(18) 0.0358(7) Uani 1 1 d . . .
H17′ H -0.1020 -0.1807 0.1805 0.043 Uiso 1 1 calc R . .
C17 C 0.1904(3) -0.5961(2) 0.40779(19) 0.0426(8) Uani 1 1 d . . .
H17 H 0.1327 -0.6357 0.4068 0.051 Uiso 1 1 calc R . .
C18′ C 0.0105(3) -0.12023(17) 0.07754(18) 0.0349(7) Uani 1 1 d . . .
H18′ H -0.0303 -0.1388 0.0426 0.042 Uiso 1 1 calc R . .
C18 C 0.1663(3) -0.5569(2) 0.46737(18) 0.0462(9) Uani 1 1 d . . .
H18 H 0.0918 -0.5691 0.5079 0.055 Uiso 1 1 calc R . .
C19′ C 0.1134(3) -0.06661(17) 0.04684(16) 0.0309(6) Uani 1 1 d . . .
H19′ H 0.1420 -0.0474 -0.0093 0.037 Uiso 1 1 calc R . .
C19 C 0.2521(3) -0.4994(2) 0.46759(17) 0.0382(7) Uani 1 1 d . . .
H19 H 0.2373 -0.4720 0.5084 0.046 Uiso 1 1 calc R . .
C20′ C 0.1729(2) -0.04200(15) 0.09935(15) 0.0244(5) Uani 1 1 d . . .
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C20 C 0.3596(3) -0.48259(17) 0.40755(15) 0.0303(6) Uani 1 1 d . . .
C21′ C 0.2811(2) 0.01513(15) 0.07397(15) 0.0246(5) Uani 1 1 d . . .
C21 C 0.4593(3) -0.42388(17) 0.40159(15) 0.0305(6) Uani 1 1 d . . .
C22′ C 0.3287(3) 0.05551(16) -0.00524(16) 0.0293(6) Uani 1 1 d . . .
H22′ H 0.2934 0.0461 -0.0474 0.035 Uiso 1 1 calc R . .
C22 C 0.4565(3) -0.37767(19) 0.45514(17) 0.0388(7) Uani 1 1 d . . .
H22 H 0.3862 -0.3815 0.4984 0.047 Uiso 1 1 calc R . .
C23′ C 0.4281(3) 0.10964(17) -0.02237(16) 0.0323(6) Uani 1 1 d . . .
H23′ H 0.4616 0.1378 -0.0763 0.039 Uiso 1 1 calc R . .
C23 C 0.5572(3) -0.3260(2) 0.44501(18) 0.0434(8) Uani 1 1 d . . .
H23 H 0.5577 -0.2951 0.4819 0.052 Uiso 1 1 calc R . .
C24′ C 0.4781(3) 0.12210(17) 0.04010(17) 0.0320(6) Uani 1 1 d . . .
H24′ H 0.5468 0.1586 0.0297 0.038 Uiso 1 1 calc R . .
C24 C 0.6570(3) -0.31982(19) 0.38048(19) 0.0403(7) Uani 1 1 d . . .
H24 H 0.7264 -0.2843 0.3723 0.048 Uiso 1 1 calc R . .
C25′ C 0.4268(3) 0.08066(16) 0.11766(16) 0.0295(6) Uani 1 1 d . . .
H25′ H 0.4613 0.0896 0.1603 0.035 Uiso 1 1 calc R . .
C25 C 0.6544(3) -0.36630(17) 0.32783(17) 0.0327(6) Uani 1 1 d . . .
H25 H 0.7225 -0.3614 0.2832 0.039 Uiso 1 1 calc R . .

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0.00095(14)
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0.00312(13)
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Cl2 0.0382(4) 0.0322(4) 0.0405(4) -0.0039(3) -0.0057(3) -0.0010(3)
Cl3 0.0444(4) 0.0493(5) 0.0304(4) -0.0061(3) -0.0043(3) 0.0066(3)
Cl4 0.0393(4) 0.0420(4) 0.0377(4) -0.0181(3) -0.0094(3) 0.0030(3)
O11 0.087(2) 0.0538(17) 0.117(3) -0.0310(17) -0.053(2) 0.0182(15)
O12 0.150(3) 0.0675(19) 0.0501(17) -0.0005(14) -0.0371(19) -0.037(2)
O13 0.0750(18) 0.0591(16) 0.0767(19) -0.0378(15) 0.0083(15) -0.0186(14)
O14 0.126(3) 0.089(2) 0.0461(16) -0.0376(16) -0.0055(17) 0.001(2)
O21 0.078(2) 0.112(3) 0.145(3) -0.061(3) -0.063(2) 0.0074(19)
O22 0.0468(14) 0.0398(14) 0.118(2) -0.0254(15) 0.0169(15) -0.0034(11)
O23 0.0454(17) 0.131(3) 0.106(3) 0.042(2) -0.0006(17) 0.0041(18)
O24 0.0513(14) 0.0578(15) 0.0442(13) -0.0189(11) -0.0034(11) -0.0190(11)
O31 0.111(2) 0.0416(15) 0.090(2) -0.0263(15) 0.0474(19) -0.0226(15)
O32 0.0719(17) 0.0403(13) 0.0499(14) -0.0002(11) 0.0060(13) -0.0047(12)
O33 0.169(3) 0.0557(17) 0.0393(15) -0.0050(12) -0.0388(18) 0.0068(19)
O34 0.0428(14) 0.0780(19) 0.145(3) -0.064(2) -0.0425(17) 0.0182(13)
O41 0.084(2) 0.0699(19) 0.073(2) -0.0056(16) 0.0247(17) -0.0189(16)
O42 0.0400(14) 0.0769(19) 0.088(2) -0.0295(16) -0.0095(13) -0.0074(13)
O43 0.0725(16) 0.0443(13) 0.0343(12) -0.0091(10) -0.0086(11) -0.0005(12)
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O61 0.0364(11) 0.0369(11) 0.0320(11) -0.0108(9) -0.0004(9) -0.0034(9)
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O1′ 0.0347(10) 0.0240(9) 0.0271(9) -0.0094(7) -0.0087(8) 0.0009(8)
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C2′ 0.0340(15) 0.0362(16) 0.0424(17) -0.0183(13) -0.0093(13) 0.0030(12)
C3′ 0.029(2) 0.032(2) 0.038(2) -0.0094(16) -0.0127(18) 0.0010(16)
C30′ 0.025(17) 0.20(4) 0.13(3) -0.14(3) 0.006(18) -0.04(2)
C2 0.0248(14) 0.0343(16) 0.0296(15) -0.0037(12) -0.0027(12) 0.0036(12)
C3 0.0313(16) 0.0427(18) 0.0339(16) -0.0139(14) -0.0037(13) 0.0038(13)
C30 0.04(6) 0.00(4) 0.00(4) -0.01(3) -0.03(4) -0.01(3)
C4′ 0.063(2) 0.059(2) 0.071(3) -0.031(2) -0.037(2) 0.0012(19)
C5′ 0.044(2) 0.057(2) 0.084(3) -0.020(2) -0.034(2) 0.0036(17)
C40′ 0.063(2) 0.059(2) 0.071(3) -0.031(2) -0.037(2) 0.0012(19)
C50′ 0.044(2) 0.057(2) 0.084(3) -0.020(2) -0.034(2) 0.0036(17)
C4 0.0337(17) 0.059(2) 0.0408(18) -0.0166(16) 0.0038(14) -0.0005(15)
C5 0.0299(16) 0.055(2) 0.057(2) -0.0250(17) -0.0073(15) 0.0067(14)
C40 0.0337(17) 0.059(2) 0.0408(18) -0.0166(16) 0.0038(14) -0.0005(15)
C50 0.0299(16) 0.055(2) 0.057(2) -0.0250(17) -0.0073(15) 0.0067(14)
C6′ 0.0421(16) 0.0325(15) 0.0295(14) -0.0041(12) -0.0093(13) -0.0063(13)
C6 0.0322(14) 0.0242(13) 0.0301(14) -0.0059(11) 0.0024(12) 0.0012(11)
C7′ 0.055(2) 0.0406(17) 0.0314(16) 0.0030(13) -0.0162(15) -0.0168(15)
C7 0.0388(16) 0.0255(14) 0.0427(17) -0.0138(13) 0.0064(13) -0.0017(12)
C8′ 0.0476(19) 0.067(2) 0.0239(15) -0.0033(15) -0.0011(14) -0.0242(17)
C8 0.0465(18) 0.0356(16) 0.0382(16) -0.0189(13) 0.0017(14) -0.0087(13)
C9′ 0.0353(16) 0.062(2) 0.0288(15) -0.0119(14) -0.0023(13) -0.0088(15)
C9 0.0365(15) 0.0342(15) 0.0321(15) -0.0122(12) -0.0024(12) -0.0043(12)
C10′ 0.0284(14) 0.0447(17) 0.0243(13) -0.0126(12) -0.0052(11) -0.0038(12)
C10 0.0262(13) 0.0248(13) 0.0234(13) -0.0066(10) 0.0010(10) -0.0034(10)
C11′ 0.0278(14) 0.0443(17) 0.0267(14) -0.0151(12) -0.0071(11) 0.0033(12)
C11 0.0249(13) 0.0258(13) 0.0209(12) -0.0055(10) 0.0003(10) -0.0028(10)
C12′ 0.0370(17) 0.060(2) 0.0373(17) -0.0256(15) -0.0027(14) 0.0060(15)
C12 0.0349(15) 0.0327(15) 0.0288(14) -0.0085(11) -0.0101(12) -0.0028(12)
C13′ 0.0427(18) 0.051(2) 0.056(2) -0.0299(17) -0.0137(16) 0.0187(15)
C13 0.0338(15) 0.0324(15) 0.0305(14) -0.0028(12) -0.0104(12) 0.0035(12)
C14′ 0.0434(17) 0.0345(16) 0.0501(19) -0.0193(14) -0.0188(15) 0.0099(13)
C14 0.0314(14) 0.0221(13) 0.0295(14) -0.0042(11) -0.0030(11) 0.0029(11)
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C23 0.062(2) 0.0417(18) 0.0342(16) -0.0205(14) -0.0219(15) 0.0173(16)

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C25’ 0.0313(14) 0.0277(14) 0.0305(14) -0.0083(11) -0.0085(12) 0.0002(11)
C25 0.0347(15) 0.0321(15) 0.0326(15) -0.0112(12) -0.0091(12) 0.0052(12)

_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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Co1 N4’ 1.950(2) .
Co1 N5’ 1.957(2) .
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Co2 N3 1.935(2) .
Co2 N2 1.943(2) .
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Co2 N5 1.957(2) .
Co2 N1 1.957(2) .
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Cl4 O24 1.451(2) . ?
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O2’ C1’ 1.213(3) .
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N1’ C2’ 1.489(3) .
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N3 C15 1.348(3) . ?
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N4 Co2 N3 C11 -88.55(18) . . . . ?
N5 Co2 N3 C11 -171.87(17) . . . . ?
N1 Co2 N3 C11 91.54(17) . . . . ?
O1' Co1 N3' C15' 141.9(13) . . . . ?
N2' Co1 N3' C15' 179.1(2) . . . . ?
N1' Co1 N3' C15' 91.2(2) . . . . ?
N4' Co1 N3' C15' -88.8(2) . . . . ?
N5' Co1 N3' C15' -5.1(2) . . . . ?
O1' Co1 N3' C11' -36.3(15) . . . . ?
N2' Co1 N3' C11' 0.93(18) . . . . ?
N1' Co1 N3' C11' -86.97(19) . . . . ?
N4' Co1 N3' C11' 92.97(19) . . . . ?
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N5′ Co1 N3′ C11′ 176.75(18) . . . . ?
O1 Co2 N4 C16 -89.2(2) . . . . ?
N3 Co2 N4 C16 86.9(2) . . . . ?
N2 Co2 N4 C16 3.7(2) . . . . ?
N5 Co2 N4 C16 -178.5(2) . . . . ?
N1 Co2 N4 C16 -93.9(8) . . . . ?
O1 Co2 N4 C20 86.10(18) . . . . ?
N3 Co2 N4 C20 -97.78(18) . . . . ?
N2 Co2 N4 C20 178.99(17) . . . . ?
N5 Co2 N4 C20 -3.20(17) . . . . ?
N1 Co2 N4 C20 81.5(8) . . . . ?
O1′ Co1 N4′ C16′ 93.3(2) . . . . ?
N2′ Co1 N4′ C16′ -0.7(2) . . . . ?
N3′ Co1 N4′ C16′ -84.0(2) . . . . ?
N1′ Co1 N4′ C16′ 95.5(9) . . . . ?
N5′ Co1 N4′ C16′ -178.4(2) . . . . ?
O1′ Co1 N4′ C20′ -81.12(17) . . . . ?
N2′ Co1 N4′ C20′ -175.09(18) . . . . ?
N3′ Co1 N4′ C20′ 101.66(18) . . . . ?
N1′ Co1 N4′ C20′ -78.9(9) . . . . ?
N5′ Co1 N4′ C20′ 7.18(17) . . . . ?
O1 Co2 N5 C25 92.3(2) . . . . ?
N3 Co2 N5 C25 -88.7(2) . . . . ?
N2 Co2 N5 C25 -146.2(12) . . . . ?
N4 Co2 N5 C25 -179.9(2) . . . . ?
N1 Co2 N5 C25 6.8(2) . . . . ?
O1 Co2 N5 C21 -84.83(17) . . . . ?
N3 Co2 N5 C21 94.14(17) . . . . ?
N2 Co2 N5 C21 36.7(13) . . . . ?
N4 Co2 N5 C21 3.01(17) . . . . ?
N1 Co2 N5 C21 -170.33(17) . . . . ?
O1′ Co1 N5′ C25′ -95.4(2) . . . . ?
N2′ Co1 N5′ C25′ 146.8(11) . . . . ?
N3′ Co1 N5′ C25′ 82.6(2) . . . . ?
N1′ Co1 N5′ C25′ -9.9(2) . . . . ?
N4′ Co1 N5′ C25′ 176.3(2) . . . . ?
O1′ Co1 N5′ C21′ 82.85(17) . . . . ?
N2′ Co1 N5′ C21′ -35.0(12) . . . . ?
N3′ Co1 N5′ C21′ -99.11(18) . . . . ?
N1′ Co1 N5′ C21′ 168.40(17) . . . . ?
N4′ Co1 N5′ C21′ -5.45(17) . . . . ?
Co1 O1′ C1′ O2′ -173.7(2) . . . . ?
Co1 O1′ C1′ C2′ 4.4(3) . . . . ?
Co2 O1 C1 O2 -179.0(2) . . . . ?
Co2 O1 C1 C2 2.0(3) . . . . ?
Co1 N1′ C2′ C30′ -166(3) . . . . ?
Co1 N1′ C2′ C3′ -140.0(3) . . . . ?
Co1 N1′ C2′ C1′ -13.9(3) . . . . ?
O2′ C1′ C2′ C30′ -21(2) . . . . ?
O1′ C1′ C2′ C30′ 161(2) . . . . ?
O2′ C1′ C2′ C3′ -50.0(4) . . . . ?
O1′ C1′ C2′ C3′ 131.8(3) . . . . ?
O2′ C1′ C2′ N1′ -175.3(3) . . . . ?
O1′ C1′ C2′ N1′ 6.6(3) . . . . ?
C30′ C2′ C3′ C5′ -15(3) . . . . ?
N1′ C2′ C3′ C5′ -141.8(3) . . . . ?
C1′ C2′ C3′ C5′ 94.6(4) . . . . ?
C30′ C2′ C3′ C4′ 55(3) . . . . ?
N1′ C2′ C3′ C4′ -72.5(5) . . . . ?
C1′ C2′ C3′ C4′ 163.9(3) . . . . ?
Co2 N1 C2 C30 -174(3) . . . . ?
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Co2 N1 C2 C3 139.3(2) . . . . ?
Co2 N1 C2 C1 14.2(3) . . . . ?
O2 C1 C2 C30 0(3) . . . . ?
O1 C1 C2 C30 179(3) . . . . ?
O2 C1 C2 N1 170.1(3) . . . . ?
O1 C1 C2 N1 -10.9(3) . . . . ?
O2 C1 C2 C3 45.0(4) . . . . ?
O1 C1 C2 C3 -136.0(3) . . . . ?
C30 C2 C3 C5 35(4) . . . . ?
N1 C2 C3 C5 142.5(3) . . . . ?
C1 C2 C3 C5 -94.7(3) . . . . ?
C30 C2 C3 C4 -35(4) . . . . ?
N1 C2 C3 C4 73.3(3) . . . . ?
C1 C2 C3 C4 -163.9(3) . . . . ?
C2′ C3′ C4′ C5′ -110.7(4) . . . . ?
C2′ C3′ C5′ C4′ 106.8(4) . . . . ?
C2 C3 C4 C5 109.9(3) . . . . ?
C2 C3 C5 C4 -107.5(3) . . . . ?
C10′ N2′ C6′ C7′ -0.6(4) . . . . ?
Co1 N2′ C6′ C7′ 179.1(2) . . . . ?
C10 N2 C6 C7 -0.4(4) . . . . ?
Co2 N2 C6 C7 -177.8(2) . . . . ?
N2′ C6′ C7′ C8′ 1.1(4) . . . . ?
N2 C6 C7 C8 -0.8(4) . . . . ?
C6′ C7′ C8′ C9′ -0.4(5) . . . . ?
C6 C7 C8 C9 0.6(4) . . . . ?
C7′ C8′ C9′ C10′ -0.6(5) . . . . ?
C7 C8 C9 C10 0.7(4) . . . . ?
C6′ N2′ C10′ C9′ -0.4(4) . . . . ?
Co1 N2′ C10′ C9′ 179.8(2) . . . . ?
C6′ N2′ C10′ C11′ 179.5(2) . . . . ?
Co1 N2′ C10′ C11′ -0.3(3) . . . . ?
C8′ C9′ C10′ N2′ 1.1(4) . . . . ?
C8′ C9′ C10′ C11′ -178.8(3) . . . . ?
C6 N2 C10 C9 1.7(4) . . . . ?
Co2 N2 C10 C9 179.4(2) . . . . ?
C6 N2 C10 C11 -177.8(2) . . . . ?
Co2 N2 C10 C11 -0.1(3) . . . . ?
C8 C9 C10 N2 -1.9(4) . . . . ?
C8 C9 C10 C11 177.5(3) . . . . ?
C15′ N3′ C11′ C12′ -0.7(4) . . . . ?
Co1 N3′ C11′ C12′ 177.7(2) . . . . ?
C15′ N3′ C11′ C10′ -179.7(2) . . . . ?
Co1 N3′ C11′ C10′ -1.3(3) . . . . ?
N2′ C10′ C11′ N3′ 1.1(3) . . . . ?
C9′ C10′ C11′ N3′ -179.0(3) . . . . ?
N2′ C10′ C11′ C12′ -177.9(3) . . . . ?
C9′ C10′ C11′ C12′ 2.0(5) . . . . ?
C15 N3 C11 C12 -2.0(4) . . . . ?
Co2 N3 C11 C12 174.0(2) . . . . ?
C15 N3 C11 C10 177.9(2) . . . . ?
Co2 N3 C11 C10 -6.1(3) . . . . ?
N2 C10 C11 N3 4.1(3) . . . . ?
C9 C10 C11 N3 -175.4(2) . . . . ?
N2 C10 C11 C12 -176.1(2) . . . . ?
C9 C10 C11 C12 4.5(4) . . . . ?
N3′ C11′ C12′ C13′ 0.0(4) . . . . ?
C10′ C11′ C12′ C13′ 178.9(3) . . . . ?
N3 C11 C12 C13 0.4(4) . . . . ?
C10 C11 C12 C13 -179.5(3) . . . . ?
C11′ C12′ C13′ C14′ 0.6(5) . . . . ?
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C11 C12 C13 C14 1.1(4) . . . . ?
C12' C13' C14' C15' -0.6(5) . . . . ?
C12 C13 C14 C15 -0.9(4) . . . . ?
C11' N3' C15' C14' 0.7(4) . . . . ?
Co1 N3' C15' C14' -177.4(2) . . . . ?
C13' C14' C15' N3' -0.1(4) . . . . ?
C11 N3 C15 C14 2.2(4) . . . . ?
Co2 N3 C15 C14 -173.26(19) . . . . ?
C13 C14 C15 N3 -0.8(4) . . . . ?
C20' N4' C16' C17' 1.9(4) . . . . ?
Co1 N4' C16' C17' -172.2(2) . . . . ?
C20 N4 C16 C17 0.9(4) . . . . ?
Co2 N4 C16 C17 176.0(2) . . . . ?
N4' C16' C17' C18' 0.1(4) . . . . ?
N4 C16 C17 C18 -0.5(4) . . . . ?
C16' C17' C18' C19' -1.8(4) . . . . ?
C16 C17 C18 C19 -0.1(4) . . . . ?
C17' C18' C19' C20' 1.4(4) . . . . ?
C17 C18 C19 C20 0.3(4) . . . . ?
C16' N4' C20' C19' -2.4(4) . . . . ?
Co1 N4' C20' C19' 172.58(19) . . . . ?
C16' N4' C20' C21' 177.6(2) . . . . ?
Co1 N4' C20' C21' -7.5(3) . . . . ?
C18' C19' C20' N4' 0.7(4) . . . . ?
C18' C19' C20' C21' -179.2(2) . . . . ?
C16 N4 C20 C19 -0.7(4) . . . . ?
Co2 N4 C20 C19 -176.40(19) . . . . ?
C16 N4 C20 C21 178.5(2) . . . . ?
Co2 N4 C20 C21 2.8(3) . . . . ?
C18 C19 C20 N4 0.1(4) . . . . ?
C18 C19 C20 C21 -179.0(2) . . . . ?
C25' N5' C21' C22' -0.7(4) . . . . ?
Co1 N5' C21' C22' -179.17(19) . . . . ?
C25' N5' C21' C20' -178.7(2) . . . . ?
Co1 N5' C21' C20' 2.9(3) . . . . ?
N4' C20' C21' N5' 3.1(3) . . . . ?
C19' C20' C21' N5' -177.0(2) . . . . ?
N4' C20' C21' C22' -174.9(2) . . . . ?
C19' C20' C21' C22' 5.1(4) . . . . ?
C25 N5 C21 C22 -0.1(4) . . . . ?
Co2 N5 C21 C22 177.26(19) . . . . ?
C25 N5 C21 C20 -179.7(2) . . . . ?
Co2 N5 C21 C20 -2.3(3) . . . . ?
N4 C20 C21 N5 -0.3(3) . . . . ?
C19 C20 C21 N5 178.9(2) . . . . ?
N4 C20 C21 C22 -179.8(2) . . . . ?
C19 C20 C21 C22 -0.7(4) . . . . ?
N5' C21' C22' C23' 0.4(4) . . . . ?
C20' C21' C22' C23' 178.2(2) . . . . ?
N5 C21 C22 C23 -1.2(4) . . . . ?
C20 C21 C22 C23 178.3(2) . . . . ?
C21' C22' C23' C24' 0.2(4) . . . . ?
C21 C22 C23 C24 1.6(4) . . . . ?
C22' C23' C24' C25' -0.4(4) . . . . ?
C22 C23 C24 C25 -0.6(4) . . . . ?
C21' N5' C25' C24' 0.4(4) . . . . ?
Co1 N5' C25' C24' 178.6(2) . . . . ?
C23' C24' C25' N5' 0.2(4) . . . . ?
C21 N5 C25 C24 1.2(4) . . . . ?
Co2 N5 C25 C24 -175.8(2) . . . . ?
C23 C24 C25 N5 -0.8(4) . . . . ?
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_diffrn_reflns_theta_full              26.45
_diffrn_measured_fraction_theta_full   0.982
_refine_diff_density_max    1.147
_refine_diff_density_min   -0.733
_refine_diff_density_rms    0.067
#=============================================================================
===
#                          END of CIF
#=============================================================================
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