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data_p21c

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 'C'  'C'   0.0033   0.0016
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 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0061   0.0033
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 'Cl'  'Cl'   0.1484   0.1585
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Rh'  'Rh'  -1.1178   0.9187
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 'x, y, z'
 '-x, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

_cell_length_a                    11.912(2)
_cell_length_b                    8.4318(17)
_cell_length_c                    17.051(3)
_cell_angle_alpha                 90.00
_cell_angle_beta                  96.14(3)
_cell_angle_gamma                 90.00
_cell_volume                      1702.7(6)
_cell_formula_units_Z             4
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;
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;

_diffrn_ambient_temperature       293(2)
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_refine_special_details
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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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 'calc w=1/[\s^2^(Fo^2^)+(0.0264P)^2^+0.5696P] where P=(Fo^2^+2Fc^2^)/3'
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Rh1 Rh 0.771451(17) 0.29440(2) 0.402708(12) 0.02396(8) Uani 1 1 d . . .
Cl2 Cl 0.72816(6) 0.54759(9) 0.46324(5) 0.03792(18) Uani 1 1 d . . .
Cl1 Cl 0.84994(6) 0.43425(10) 0.29846(5) 0.04127(19) Uani 1 1 d . . .
```

```
N1 N 0.60990(18) 0.2840(3) 0.33118(13) 0.0265(5) Uani 1 1 d . . .
N2 N 0.5046(2) 0.3384(3) 0.43503(14) 0.0362(6) Uani 1 1 d . . .
H2 H 0.5010 0.2746 0.4836 0.043 Uiso 1 1 d R . .
H1 H 0.5687 0.3919 0.4498 0.043 Uiso 1 1 d R . .
C16 C 0.2984(3) 0.2423(4) 0.3486(2) 0.0416(8) Uani 1 1 d . . .
H11A H 0.3054 0.1902 0.3989 0.062 Uiso 1 1 calc R . .
H11B H 0.2415 0.1901 0.3136 0.062 Uiso 1 1 calc R . .
H11C H 0.2773 0.3510 0.3550 0.062 Uiso 1 1 calc R . .
C3 C 0.9250(2) 0.1572(4) 0.43081(19) 0.0370(7) Uani 1 1 d . . .
C5 C 0.7774(2) 0.1556(3) 0.50852(17) 0.0322(6) Uani 1 1 d . . .
C1 C 0.7469(2) 0.0562(3) 0.44249(17) 0.0308(6) Uani 1 1 d . . .
C12 C 0.4092(2) 0.2355(3) 0.31441(17) 0.0296(6) Uani 1 1 d . . .
C11 C 0.5087(2) 0.2880(3) 0.35972(16) 0.0262(6) Uani 1 1 d . . .
C10 C 0.7134(3) 0.1840(4) 0.5775(2) 0.0502(9) Uani 1 1 d . . .
H18A H 0.7171 0.2945 0.5911 0.075 Uiso 1 1 calc R . .
H18B H 0.7457 0.1221 0.6215 0.075 Uiso 1 1 calc R . .
H18C H 0.6360 0.1537 0.5643 0.075 Uiso 1 1 calc R . .
C2 C 0.8363(2) 0.0603(3) 0.39228(18) 0.0339(7) Uani 1 1 d . . .
C13 C 0.4181(3) 0.1783(3) 0.24003(18) 0.0352(7) Uani 1 1 d . . .
H7 H 0.3545 0.1394 0.2097 0.042 Uiso 1 1 calc R . .
C4 C 0.8889(3) 0.2186(3) 0.50120(19) 0.0360(7) Uani 1 1 d . . .
C8 C 1.0361(3) 0.1865(4) 0.4006(3) 0.0572(10) Uani 1 1 d . . .
H20A H 1.0816 0.0925 0.4072 0.086 Uiso 1 1 calc R . .
H20B H 1.0740 0.2722 0.4296 0.086 Uiso 1 1 calc R . .
H20C H 1.0243 0.2138 0.3457 0.086 Uiso 1 1 calc R . .
C14 C 0.5220(3) 0.1785(4) 0.21000(17) 0.0361(7) Uani 1 1 d . . .
H8 H 0.5284 0.1423 0.1592 0.043 Uiso 1 1 calc R . .
C15 C 0.6142(2) 0.2325(3) 0.25638(17) 0.0307(6) Uani 1 1 d . . .
H9 H 0.6833 0.2341 0.2357 0.037 Uiso 1 1 calc R . .
C9 C 0.9542(3) 0.3218(4) 0.5616(2) 0.0576(10) Uani 1 1 d . . .
H19A H 1.0275 0.3431 0.5455 0.086 Uiso 1 1 calc R . .
H19B H 0.9622 0.2685 0.6116 0.086 Uiso 1 1 calc R . .
H19C H 0.9146 0.4199 0.5662 0.086 Uiso 1 1 calc R . .
C6 C 0.6404(3) -0.0384(4) 0.4269(2) 0.0441(8) Uani 1 1 d . . .
H17A H 0.5862 -0.0017 0.4605 0.066 Uiso 1 1 calc R . .
H17B H 0.6565 -0.1484 0.4374 0.066 Uiso 1 1 calc R . .
H17C H 0.6104 -0.0258 0.3727 0.066 Uiso 1 1 calc R . .
C7 C 0.8401(3) -0.0332(4) 0.3185(2) 0.0573(10) Uani 1 1 d . . .
H21A H 0.7652 -0.0423 0.2917 0.086 Uiso 1 1 calc R . .
H21B H 0.8695 -0.1371 0.3313 0.086 Uiso 1 1 calc R . .
H21C H 0.8879 0.0195 0.2848 0.086 Uiso 1 1 calc R . .

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Cl2 0.0356(4) 0.0308(4) 0.0468(4) -0.0094(3) 0.0015(3) 0.0019(3)
Cl1 0.0325(4) 0.0515(5) 0.0403(4) 0.0135(4) 0.0062(3) -0.0036(3)
N1 0.0222(12) 0.0314(13) 0.0253(12) 0.0003(10) -0.0005(9) 0.0009(10)
```

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N2 0.0315(14) 0.0485(16) 0.0290(13) -0.0059(12) 0.0052(10) -0.0070(12)
C16 0.0270(16) 0.055(2) 0.0420(18) -0.0027(16) 0.0018(13) -0.0050(14)
C3 0.0266(15) 0.0401(17) 0.0440(18) 0.0112(15) 0.0030(13) 0.0106(13)
C5 0.0362(16) 0.0301(15) 0.0305(15) 0.0072(13) 0.0040(12) 0.0059(13)
C1 0.0333(16) 0.0242(14) 0.0346(16) 0.0056(13) 0.0022(12) 0.0069(12)
C12 0.0276(15) 0.0284(14) 0.0327(15) 0.0030(12) 0.0018(12) -0.0025(12)
C11 0.0245(14) 0.0253(14) 0.0289(14) 0.0012(12) 0.0034(11) -0.0001(11)
C10 0.068(2) 0.051(2) 0.0333(18) 0.0053(16) 0.0131(16) 0.0054(18)
C2 0.0330(16) 0.0316(16) 0.0370(16) 0.0024(13) 0.0035(12) 0.0090(13)
C13 0.0304(16) 0.0368(17) 0.0365(16) -0.0005(14) -0.0042(12) -0.0073(13)
C4 0.0322(17) 0.0327(16) 0.0402(17) 0.0089(14) -0.0093(13) 0.0025(13)
C8 0.0290(18) 0.063(2) 0.081(3) 0.017(2) 0.0122(18) 0.0116(17)
C14 0.0392(17) 0.0429(18) 0.0255(15) -0.0069(13) 0.0004(12) -0.0021(14)
C15 0.0286(16) 0.0379(16) 0.0261(14) -0.0004(13) 0.0048(12) 0.0021(13)
C9 0.057(2) 0.059(2) 0.050(2) -0.0008(19) -0.0248(18) -0.0026(18)
C6 0.045(2) 0.0313(16) 0.055(2) 0.0053(15) 0.0032(16) -0.0082(15)
C7 0.069(3) 0.053(2) 0.050(2) -0.0142(19) 0.0069(18) 0.0230(19)

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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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Rh1 C5 2.145(3) . ?
Rh1 C1 2.150(3) . ?
Rh1 C4 2.164(3) . ?
Rh1 N1 2.167(2) . ?
Rh1 C3 2.173(3) . ?
Rh1 Cl1 2.4040(9) . ?
Rh1 Cl2 2.4501(8) . ?
N1 C11 1.348(3) . ?
N1 C15 1.353(4) . ?
N2 C11 1.358(4) . ?
N2 H2 0.9920 . ?
N2 H1 0.8999 . ?
C16 C12 1.500(4) . ?
C16 H11A 0.9600 . ?
C16 H11B 0.9600 . ?
C16 H11C 0.9600 . ?
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C3 C4 1.415(4) . ?
C3 C2 1.437(4) . ?
C3 C8 1.491(4) . ?
C5 C1 1.420(4) . ?
C5 C4 1.448(4) . ?
C5 C10 1.488(4) . ?
C1 C2 1.437(4) . ?
C1 C6 1.497(4) . ?
C12 C13 1.372(4) . ?
C12 C11 1.414(4) . ?
C10 H18A 0.9600 . ?
C10 H18B 0.9600 . ?
C10 H18C 0.9600 . ?
C2 C7 1.490(4) . ?
C13 C14 1.389(4) . ?
C13 H7 0.9300 . ?
C4 C9 1.500(4) . ?
C8 H20A 0.9600 . ?
C8 H20B 0.9600 . ?
C8 H20C 0.9600 . ?
C14 C15 1.361(4) . ?
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C15 H9 0.9300 . ?
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C9 H19C 0.9600 . ?
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C2 Rh1 C1 39.19(11) . . ?
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C5 Rh1 C4 39.26(11) . . ?
C1 Rh1 C4 65.03(11) . . ?
C2 Rh1 N1 102.91(10) . . ?
C5 Rh1 N1 113.51(10) . . ?
C1 Rh1 N1 89.83(10) . . ?
C4 Rh1 N1 152.40(10) . . ?
C2 Rh1 C3 38.97(11) . . ?
C5 Rh1 C3 64.71(11) . . ?
C1 Rh1 C3 64.73(11) . . ?
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N1 Rh1 C3 141.09(11) . . ?
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C5 Rh1 Cl1 155.34(8) . . ?
C1 Rh1 Cl1 140.20(8) . . ?
C4 Rh1 Cl1 116.64(9) . . ?
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C1 Rh1 Cl2 129.74(8) . . ?
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C15 N1 Rh1 115.01(18) . . ?
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H2 N2 H1 98.5 . . ?
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C12 C16 H11B 109.5 . . ?
H11A C16 H11B 109.5 . . ?
C12 C16 H11C 109.5 . . ?
H11A C16 H11C 109.5 . . ?
H11B C16 H11C 109.5 . . ?
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C4 C3 C8 126.4(3) . . ?
C2 C3 C8 124.9(3) . . ?
C4 C3 Rh1 70.62(16) . . ?
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C1 C5 C4 107.9(3) . . ?
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C2 C1 Rh1 69.79(16) . . ?
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C11 C12 C16 119.8(3) . . ?
N1 C11 N2 118.2(2) . . ?
N1 C11 C12 121.6(3) . . ?
N2 C11 C12 120.1(3) . . ?
C5 C10 H18A 109.5 . . ?
C5 C10 H18B 109.5 . . ?
H18A C10 H18B 109.5 . . ?
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C5 C10 H18C 109.5 . . ?
H18A C10 H18C 109.5 . . ?
H18B C10 H18C 109.5 . . ?
C1 C2 C3 107.3(3) . . ?
C1 C2 C7 125.5(3) . . ?
C3 C2 C7 126.9(3) . . ?
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C7 C2 Rh1 127.1(2) . . ?
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C3 C4 C5 107.7(3) . . ?
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C5 C4 Rh1 69.66(16) . . ?
C9 C4 Rh1 127.3(2) . . ?
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C3 C8 H20B 109.5 . . ?
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C3 C8 H20C 109.5 . . ?
H20A C8 H20C 109.5 . . ?
H20B C8 H20C 109.5 . . ?
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C4 C9 H19C 109.5 . . ?
H19A C9 H19C 109.5 . . ?
H19B C9 H19C 109.5 . . ?
C1 C6 H17A 109.5 . . ?
C1 C6 H17B 109.5 . . ?
H17A C6 H17B 109.5 . . ?
C1 C6 H17C 109.5 . . ?
H17A C6 H17C 109.5 . . ?
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C3 Rh1 N1 C11 119.5(2) . . . . ?
Cl1 Rh1 N1 C11 -147.2(2) . . . . ?
Cl2 Rh1 N1 C11 -57.3(2) . . . . ?
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C4 Rh1 N1 C15 -114.7(3) . . . . ?
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Cl2 Rh1 N1 C15 139.01(19) . . . . ?
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Cl2 Rh1 C3 C4 41.0(2) . . . . ?
C5 Rh1 C3 C2 81.70(19) . . . . ?
C1 Rh1 C3 C2 38.82(17) . . . . ?
C4 Rh1 C3 C2 119.9(3) . . . . ?
N1 Rh1 C3 C2 -15.0(3) . . . . ?
Cl1 Rh1 C3 C2 -107.45(17) . . . . ?
Cl2 Rh1 C3 C2 160.93(14) . . . . ?
C2 Rh1 C3 C8 118.6(4) . . . . ?
C5 Rh1 C3 C8 -159.7(4) . . . . ?
C1 Rh1 C3 C8 157.4(3) . . . . ?
C4 Rh1 C3 C8 -121.5(4) . . . . ?
N1 Rh1 C3 C8 103.6(3) . . . . ?
Cl1 Rh1 C3 C8 11.2(3) . . . . ?
Cl2 Rh1 C3 C8 -80.4(3) . . . . ?
C2 Rh1 C5 C1 -37.37(16) . . . . ?
C4 Rh1 C5 C1 -117.6(2) . . . . ?
N1 Rh1 C5 C1 56.63(18) . . . . ?
C3 Rh1 C5 C1 -80.51(18) . . . . ?
Cl1 Rh1 C5 C1 -102.9(2) . . . . ?
Cl2 Rh1 C5 C1 153.06(15) . . . . ?
C2 Rh1 C5 C4 80.23(18) . . . . ?
C1 Rh1 C5 C4 117.6(2) . . . . ?
N1 Rh1 C5 C4 174.23(16) . . . . ?
C3 Rh1 C5 C4 37.09(18) . . . . ?
Cl1 Rh1 C5 C4 14.7(3) . . . . ?
Cl2 Rh1 C5 C4 -89.33(16) . . . . ?
C2 Rh1 C5 C10 -160.7(3) . . . . ?
C1 Rh1 C5 C10 -123.4(4) . . . . ?
C4 Rh1 C5 C10 119.0(4) . . . . ?
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N1 Rh1 C5 C10 -66.7(3) . . . . ?
C3 Rh1 C5 C10 156.1(3) . . . . ?
Cl1 Rh1 C5 C10 133.7(2) . . . . ?
Cl2 Rh1 C5 C10 29.7(3) . . . . ?
C4 C5 C1 C2 -2.0(3) . . . . ?
C10 C5 C1 C2 -177.6(3) . . . . ?
Rh1 C5 C1 C2 59.78(19) . . . . ?
C4 C5 C1 C6 177.7(3) . . . . ?
C10 C5 C1 C6 2.1(5) . . . . ?
Rh1 C5 C1 C6 -120.5(3) . . . . ?
C4 C5 C1 Rh1 -61.8(2) . . . . ?
C10 C5 C1 Rh1 122.6(3) . . . . ?
C2 Rh1 C1 C5 119.0(2) . . . . ?
C4 Rh1 C1 C5 38.21(17) . . . . ?
N1 Rh1 C1 C5 -130.02(17) . . . . ?
C3 Rh1 C1 C5 80.45(18) . . . . ?
Cl1 Rh1 C1 C5 140.55(14) . . . . ?
Cl2 Rh1 C1 C5 -35.8(2) . . . . ?
C5 Rh1 C1 C2 -119.0(2) . . . . ?
C4 Rh1 C1 C2 -80.84(19) . . . . ?
N1 Rh1 C1 C2 110.93(17) . . . . ?
C3 Rh1 C1 C2 -38.60(17) . . . . ?
Cl1 Rh1 C1 C2 21.5(2) . . . . ?
Cl2 Rh1 C1 C2 -154.88(14) . . . . ?
C2 Rh1 C1 C6 -119.3(3) . . . . ?
C5 Rh1 C1 C6 121.6(3) . . . . ?
C4 Rh1 C1 C6 159.8(3) . . . . ?
N1 Rh1 C1 C6 -8.4(3) . . . . ?
C3 Rh1 C1 C6 -157.9(3) . . . . ?
Cl1 Rh1 C1 C6 -97.8(3) . . . . ?
Cl2 Rh1 C1 C6 85.8(3) . . . . ?
C15 N1 C11 N2 179.4(3) . . . . ?
Rh1 N1 C11 N2 16.2(3) . . . . ?
C15 N1 C11 C12 2.0(4) . . . . ?
Rh1 N1 C11 C12 -161.3(2) . . . . ?
C13 C12 C11 N1 0.6(4) . . . . ?
C16 C12 C11 N1 -179.9(3) . . . . ?
C13 C12 C11 N2 -176.8(3) . . . . ?
C16 C12 C11 N2 2.6(4) . . . . ?
C5 C1 C2 C3 3.1(3) . . . . ?
C6 C1 C2 C3 -176.7(3) . . . . ?
Rh1 C1 C2 C3 63.3(2) . . . . ?
C5 C1 C2 C7 177.2(3) . . . . ?
C6 C1 C2 C7 -2.6(5) . . . . ?
Rh1 C1 C2 C7 -122.6(3) . . . . ?
C5 C1 C2 Rh1 -60.23(19) . . . . ?
C6 C1 C2 Rh1 120.0(3) . . . . ?
C4 C3 C2 C1 -3.0(3) . . . . ?
C8 C3 C2 C1 176.9(3) . . . . ?
Rh1 C3 C2 C1 -62.66(19) . . . . ?
C4 C3 C2 C7 -177.0(3) . . . . ?
C8 C3 C2 C7 2.9(5) . . . . ?
Rh1 C3 C2 C7 123.4(3) . . . . ?
C4 C3 C2 Rh1 59.7(2) . . . . ?
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C8 C3 C2 Rh1 -120.4(3) . . . . ?
C5 Rh1 C2 C1 36.82(17) . . . . ?
C4 Rh1 C2 C1 80.18(18) . . . . ?
N1 Rh1 C2 C1 -73.39(18) . . . . ?
C3 Rh1 C2 C1 116.2(3) . . . . ?
Cl1 Rh1 C2 C1 -166.09(15) . . . . ?
Cl2 Rh1 C2 C1 67.4(3) . . . . ?
C5 Rh1 C2 C3 -79.41(19) . . . . ?
C1 Rh1 C2 C3 -116.2(3) . . . . ?
C4 Rh1 C2 C3 -36.05(18) . . . . ?
N1 Rh1 C2 C3 170.38(17) . . . . ?
Cl1 Rh1 C2 C3 77.68(17) . . . . ?
Cl2 Rh1 C2 C3 -48.8(3) . . . . ?
C5 Rh1 C2 C7 157.5(3) . . . . ?
C1 Rh1 C2 C7 120.7(4) . . . . ?
C4 Rh1 C2 C7 -159.1(3) . . . . ?
N1 Rh1 C2 C7 47.3(3) . . . . ?
C3 Rh1 C2 C7 -123.1(4) . . . . ?
Cl1 Rh1 C2 C7 -45.4(3) . . . . ?
Cl2 Rh1 C2 C7 -171.9(2) . . . . ?
C11 C12 C13 C14 -2.4(4) . . . . ?
C16 C12 C13 C14 178.2(3) . . . . ?
C2 C3 C4 C5 1.8(3) . . . . ?
C8 C3 C4 C5 -178.1(3) . . . . ?
Rh1 C3 C4 C5 60.5(2) . . . . ?
C2 C3 C4 C9 178.2(3) . . . . ?
C8 C3 C4 C9 -1.7(5) . . . . ?
Rh1 C3 C4 C9 -123.1(3) . . . . ?
C2 C3 C4 Rh1 -58.7(2) . . . . ?
C8 C3 C4 Rh1 121.4(3) . . . . ?
C1 C5 C4 C3 0.1(3) . . . . ?
C10 C5 C4 C3 175.9(3) . . . . ?
Rh1 C5 C4 C3 -61.5(2) . . . . ?
C1 C5 C4 C9 -176.4(3) . . . . ?
C10 C5 C4 C9 -0.6(5) . . . . ?
Rh1 C5 C4 C9 121.9(3) . . . . ?
C1 C5 C4 Rh1 61.66(19) . . . . ?
C10 C5 C4 Rh1 -122.5(3) . . . . ?
C2 Rh1 C4 C3 36.88(18) . . . . ?
C5 Rh1 C4 C3 117.9(3) . . . . ?
C1 Rh1 C4 C3 80.27(19) . . . . ?
N1 Rh1 C4 C3 106.4(3) . . . . ?
Cl1 Rh1 C4 C3 -55.35(19) . . . . ?
Cl2 Rh1 C4 C3 -147.61(17) . . . . ?
C2 Rh1 C4 C5 -80.97(18) . . . . ?
C1 Rh1 C4 C5 -37.59(16) . . . . ?
N1 Rh1 C4 C5 -11.5(3) . . . . ?
C3 Rh1 C4 C5 -117.9(3) . . . . ?
Cl1 Rh1 C4 C5 -173.20(14) . . . . ?
Cl2 Rh1 C4 C5 94.54(16) . . . . ?
C2 Rh1 C4 C9 160.5(4) . . . . ?
C5 Rh1 C4 C9 -118.5(4) . . . . ?
C1 Rh1 C4 C9 -156.1(4) . . . . ?
N1 Rh1 C4 C9 -130.0(3) . . . . ?
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C3 Rh1 C4 C9 123.7(4) . . . . ?
Cl1 Rh1 C4 C9 68.3(3) . . . . ?
Cl2 Rh1 C4 C9 -23.9(3) . . . . ?
C12 C13 C14 C15 1.6(5) . . . . ?
C11 N1 C15 C14 -2.9(4) . . . . ?
Rh1 N1 C15 C14 162.0(2) . . . . ?
C13 C14 C15 N1 1.1(5) . . . . ?

_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              26.37
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    0.582
_refine_diff_density_min   -0.771
_refine_diff_density_rms    0.074
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