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data_p21c

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 'C16 H23 Cl2 Ir N2'
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 'C'  'C'   0.0033   0.0016
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 'H'  'H'   0.0000   0.0000
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ir'  'Ir'  -1.4442   7.9887
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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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                    11.908(2)
_cell_length_b                    8.4938(17)
_cell_length_c                    17.194(3)
_cell_angle_alpha                 90.00
_cell_angle_beta                  96.42(3)
_cell_angle_gamma                 90.00
_cell_volume                      1728.1(6)
_cell_formula_units_Z             4
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_exptl_crystal_density_diffrn     1.947
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_exptl_absorpt_coefficient_mu     8.031
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;

_diffrn_ambient_temperature       293(2)
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_diffrn_reflns_limit_l_max        11
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_computing_cell_refinement        ?
_computing_data_reduction         ?
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_computing_molecular_graphics     ?
_computing_publication_material   ?

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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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_refine_ls_weighting_details
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Cl2 Cl 0.27428(11) 0.54880(15) 0.04041(8) 0.0401(3) Uani 1 1 d . . .
Cl1 Cl 0.15490(12) 0.43460(17) 0.19896(8) 0.0441(3) Uani 1 1 d . . .
```

```
N1 N 0.3905(4) 0.2862(4) 0.1667(2) 0.0284(9) Uani 1 1 d . . .
N2 N 0.4976(4) 0.3406(6) 0.0641(2) 0.0378(10) Uani 1 1 d . . .
H1 H 0.4836 0.2631 0.0323 0.045 Uiso 1 1 d R . .
H2 H 0.4481 0.4134 0.0532 0.045 Uiso 1 1 d R . .
C11 C 0.4920(4) 0.2901(5) 0.1392(3) 0.0279(10) Uani 1 1 d . . .
C12 C 0.5925(4) 0.2401(6) 0.1846(3) 0.0316(11) Uani 1 1 d . . .
C3 C 0.1153(5) 0.2202(6) -0.0039(3) 0.0390(13) Uani 1 1 d . . .
C2 C 0.2243(5) 0.1578(6) -0.0107(3) 0.0343(11) Uani 1 1 d . . .
C13 C 0.5837(5) 0.1839(6) 0.2590(3) 0.0380(12) Uani 1 1 d . . .
H7 H 0.6475 0.1474 0.2898 0.046 Uiso 1 1 calc R . .
C14 C 0.4793(5) 0.1819(6) 0.2878(3) 0.0386(12) Uani 1 1 d . . .
H8 H 0.4725 0.1458 0.3381 0.046 Uiso 1 1 calc R . .
C4 C 0.0755(5) 0.1583(6) 0.0667(3) 0.0401(13) Uani 1 1 d . . .
C16 C 0.7034(5) 0.2476(8) 0.1512(3) 0.0461(14) Uani 1 1 d . . .
H11A H 0.6982 0.1893 0.1031 0.069 Uiso 1 1 calc R . .
H11B H 0.7615 0.2031 0.1879 0.069 Uiso 1 1 calc R . .
H11C H 0.7214 0.3554 0.1413 0.069 Uiso 1 1 calc R . .
C7 C 0.2892(6) 0.1845(8) -0.0787(3) 0.0565(17) Uani 1 1 d . . .
H20A H 0.2888 0.2947 -0.0911 0.085 Uiso 1 1 calc R . .
H20B H 0.2549 0.1265 -0.1230 0.085 Uiso 1 1 calc R . .
H20C H 0.3657 0.1496 -0.0657 0.085 Uiso 1 1 calc R . .
C8 C 0.0498(7) 0.3246(8) -0.0639(4) 0.069(2) Uani 1 1 d . . .
H21A H -0.0252 0.3402 -0.0498 0.103 Uiso 1 1 calc R . .
H21B H 0.0457 0.2756 -0.1144 0.103 Uiso 1 1 calc R . .
H21C H 0.0872 0.4245 -0.0656 0.103 Uiso 1 1 calc R . .
C9 C -0.0356(6) 0.1872(8) 0.0953(5) 0.068(2) Uani 1 1 d . . .
H17A H -0.0245 0.2144 0.1498 0.102 Uiso 1 1 calc R . .
H17B H -0.0810 0.0938 0.0884 0.102 Uiso 1 1 calc R . .
H17C H -0.0732 0.2722 0.0662 0.102 Uiso 1 1 calc R . .
C10 C 0.1602(6) -0.0357(8) 0.1773(4) 0.0650(19) Uani 1 1 d . . .
H18A H 0.2350 -0.0455 0.2041 0.097 Uiso 1 1 calc R . .
H18B H 0.1308 -0.1384 0.1635 0.097 Uiso 1 1 calc R . .
H18C H 0.1122 0.0152 0.2109 0.097 Uiso 1 1 calc R . .
C15 C 0.3869(5) 0.2339(6) 0.2409(3) 0.0324(11) Uani 1 1 d . . .
H9 H 0.3175 0.2336 0.2609 0.039 Uiso 1 1 calc R . .
C1 C 0.2546(4) 0.0573(6) 0.0554(3) 0.0332(11) Uani 1 1 d . . .
C5 C 0.1641(5) 0.0600(6) 0.1049(3) 0.0365(12) Uani 1 1 d . . .
C6 C 0.3613(5) -0.0361(7) 0.0713(4) 0.0504(15) Uani 1 1 d . . .
H19A H 0.4188 0.0094 0.0434 0.076 Uiso 1 1 calc R . .
H19B H 0.3477 -0.1428 0.0543 0.076 Uiso 1 1 calc R . .
H19C H 0.3859 -0.0349 0.1264 0.076 Uiso 1 1 calc R . .

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0.00151(8)
Cl2 0.0385(7) 0.0305(6) 0.0508(7) 0.0090(6) 0.0024(6) -0.0014(6)
Cl1 0.0353(7) 0.0511(8) 0.0470(7) -0.0145(6) 0.0092(6) 0.0034(6)
```

```
N1 0.027(2) 0.027(2) 0.030(2) -0.0014(17) 0.0019(16) -0.0034(17)
N2 0.034(3) 0.048(3) 0.033(2) 0.006(2) 0.0061(18) 0.005(2)
C11 0.030(3) 0.023(2) 0.031(2) 0.001(2) 0.0057(19) 0.001(2)
C12 0.026(3) 0.032(2) 0.036(3) -0.003(2) 0.003(2) 0.002(2)
C3 0.033(3) 0.036(3) 0.045(3) -0.011(2) -0.009(2) -0.005(2)
C2 0.039(3) 0.033(2) 0.031(2) -0.006(2) 0.005(2) -0.010(2)
C13 0.036(3) 0.040(3) 0.037(3) 0.003(2) -0.003(2) 0.007(2)
C14 0.040(3) 0.044(3) 0.032(3) 0.005(2) 0.004(2) 0.005(2)
C4 0.027(3) 0.041(3) 0.053(3) -0.013(3) 0.006(2) -0.013(2)
C16 0.029(3) 0.064(4) 0.046(3) 0.002(3) 0.006(2) 0.009(3)
C7 0.075(5) 0.059(4) 0.036(3) -0.007(3) 0.010(3) -0.006(3)
C8 0.069(5) 0.061(4) 0.067(4) -0.002(3) -0.036(4) 0.005(4)
C9 0.036(4) 0.067(5) 0.102(6) -0.019(4) 0.017(4) -0.016(3)
C10 0.073(5) 0.060(4) 0.063(4) 0.015(3) 0.012(3) -0.024(4)
C15 0.031(3) 0.035(3) 0.031(3) 0.004(2) 0.007(2) -0.002(2)
C1 0.032(3) 0.026(2) 0.041(3) -0.006(2) -0.001(2) -0.001(2)
C5 0.037(3) 0.030(2) 0.042(3) -0.007(2) 0.008(2) -0.015(2)
C6 0.048(4) 0.035(3) 0.066(4) -0.007(3) 0.000(3) 0.013(3)

_geom_special_details
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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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Ir1 C5 2.146(5) . ?
Ir1 C2 2.147(5) . ?
Ir1 N1 2.149(4) . ?
Ir1 C3 2.155(5) . ?
Ir1 C4 2.181(5) . ?
Ir1 Cl1 2.4083(14) . ?
Ir1 Cl2 2.4464(13) . ?
N1 C11 1.347(6) . ?
N1 C15 1.356(6) . ?
N2 C11 1.370(6) . ?
N2 H1 0.8602 . ?
N2 H2 0.8609 . ?
C11 C12 1.418(7) . ?
C12 C13 1.380(7) . ?
C12 C16 1.499(8) . ?
```

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C3 C2 1.418(8) . ?
C3 C4 1.451(8) . ?
C3 C8 1.509(8) . ?
C2 C1 1.435(7) . ?
C2 C7 1.489(7) . ?
C13 C14 1.388(8) . ?
C13 H7 0.9300 . ?
C14 C15 1.363(7) . ?
C14 H8 0.9300 . ?
C4 C5 1.445(8) . ?
C4 C9 1.483(9) . ?
C16 H11A 0.9600 . ?
C16 H11B 0.9600 . ?
C16 H11C 0.9600 . ?
C7 H20A 0.9600 . ?
C7 H20B 0.9600 . ?
C7 H20C 0.9600 . ?
C8 H21A 0.9600 . ?
C8 H21B 0.9600 . ?
C8 H21C 0.9600 . ?
C9 H17A 0.9600 . ?
C9 H17B 0.9600 . ?
C9 H17C 0.9600 . ?
C10 C5 1.491(8) . ?
C10 H18A 0.9600 . ?
C10 H18B 0.9600 . ?
C10 H18C 0.9600 . ?
C15 H9 0.9300 . ?
C1 C5 1.446(7) . ?
C1 C6 1.498(7) . ?
C6 H19A 0.9600 . ?
C6 H19B 0.9600 . ?
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C1 Ir1 C2 39.05(19) . . ?
C5 Ir1 C2 66.06(19) . . ?
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C5 Ir1 N1 103.95(18) . . ?
C2 Ir1 N1 114.52(18) . . ?
C1 Ir1 C3 64.90(19) . . ?
C5 Ir1 C3 65.7(2) . . ?
C2 Ir1 C3 38.5(2) . . ?
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C5 Ir1 C4 39.0(2) . . ?
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C3 Ir1 C4 39.1(2) . . ?
C1 Ir1 Cl1 140.93(14) . . ?
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N1 Ir1 Cl1 88.33(11) . . ?
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C1 Ir1 Cl2 131.61(15) . . ?
C5 Ir1 Cl2 161.00(14) . . ?
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C4 Ir1 Cl2 126.23(16) . . ?
Cl1 Ir1 Cl2 87.45(5) . . ?
C11 N1 C15 117.5(4) . . ?
C11 N1 Ir1 124.9(3) . . ?
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C11 N2 H2 109.0 . . ?
H1 N2 H2 109.4 . . ?
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N2 C11 C12 119.0(5) . . ?
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C13 C12 C16 122.1(5) . . ?
C11 C12 C16 120.1(5) . . ?
C2 C3 C4 108.7(5) . . ?
C2 C3 C8 124.8(6) . . ?
C4 C3 C8 126.3(6) . . ?
C2 C3 Ir1 70.4(3) . . ?
C4 C3 Ir1 71.4(3) . . ?
C8 C3 Ir1 127.3(4) . . ?
C3 C2 C1 108.0(5) . . ?
C3 C2 C7 124.6(5) . . ?
C1 C2 C7 127.3(5) . . ?
C3 C2 Ir1 71.1(3) . . ?
C1 C2 Ir1 70.4(3) . . ?
C7 C2 Ir1 127.7(4) . . ?
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C15 C14 C13 118.7(5) . . ?
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C13 C14 H8 120.6 . . ?
C5 C4 C3 107.5(5) . . ?
C5 C4 C9 125.3(6) . . ?
C3 C4 C9 127.2(6) . . ?
C5 C4 Ir1 69.2(3) . . ?
C3 C4 Ir1 69.5(3) . . ?
C9 C4 Ir1 127.1(4) . . ?
C12 C16 H11A 109.5 . . ?
C12 C16 H11B 109.5 . . ?
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C12 C16 H11C 109.5 . . ?
H11A C16 H11C 109.5 . . ?
H11B C16 H11C 109.5 . . ?
C2 C7 H20A 109.5 . . ?
C2 C7 H20B 109.5 . . ?
H20A C7 H20B 109.5 . . ?
C2 C7 H20C 109.5 . . ?
H20A C7 H20C 109.5 . . ?
H20B C7 H20C 109.5 . . ?
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C3 C8 H21B 109.5 . . ?
H21A C8 H21B 109.5 . . ?
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H21A C8 H21C 109.5 . . ?
H21B C8 H21C 109.5 . . ?
C4 C9 H17A 109.5 . . ?
C4 C9 H17B 109.5 . . ?
H17A C9 H17B 109.5 . . ?
C4 C9 H17C 109.5 . . ?
H17A C9 H17C 109.5 . . ?
H17B C9 H17C 109.5 . . ?
C5 C10 H18A 109.5 . . ?
C5 C10 H18B 109.5 . . ?
H18A C10 H18B 109.5 . . ?
C5 C10 H18C 109.5 . . ?
H18A C10 H18C 109.5 . . ?
H18B C10 H18C 109.5 . . ?
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N1 C15 H9 118.2 . . ?
C14 C15 H9 118.2 . . ?
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C5 C1 Ir1 70.3(3) . . ?
C6 C1 Ir1 125.2(4) . . ?
C4 C5 C1 107.2(4) . . ?
C4 C5 C10 127.2(5) . . ?
C1 C5 C10 125.3(5) . . ?
C4 C5 Ir1 71.8(3) . . ?
C1 C5 Ir1 70.3(3) . . ?
C10 C5 Ir1 127.9(4) . . ?
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C1 C6 H19B 109.5 . . ?
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C5 Ir1 N1 C11 109.5(4) . . . . ?
C2 Ir1 N1 C11 39.8(4) . . . . ?
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C4 Ir1 N1 C11 120.2(4) . . . . ?
Cl1 Ir1 N1 C11 -147.2(4) . . . . ?
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C3 Ir1 N1 C15 -116.6(5) . . . . ?
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Cl2 Ir1 N1 C15 137.9(3) . . . . ?
C15 N1 C11 N2 179.2(4) . . . . ?
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N2 C11 C12 C16 1.9(7) . . . . ?
C1 Ir1 C3 C2 -37.9(3) . . . . ?
C5 Ir1 C3 C2 -81.5(3) . . . . ?
N1 Ir1 C3 C2 -8.8(6) . . . . ?
C4 Ir1 C3 C2 -118.6(5) . . . . ?
Cl1 Ir1 C3 C2 -174.1(2) . . . . ?
Cl2 Ir1 C3 C2 95.9(3) . . . . ?
C1 Ir1 C3 C4 80.7(3) . . . . ?
C5 Ir1 C3 C4 37.1(3) . . . . ?
C2 Ir1 C3 C4 118.6(5) . . . . ?
N1 Ir1 C3 C4 109.8(5) . . . . ?
Cl1 Ir1 C3 C4 -55.5(3) . . . . ?
Cl2 Ir1 C3 C4 -145.5(3) . . . . ?
C1 Ir1 C3 C8 -157.3(7) . . . . ?
C5 Ir1 C3 C8 159.1(7) . . . . ?
C2 Ir1 C3 C8 -119.4(7) . . . . ?
N1 Ir1 C3 C8 -128.2(6) . . . . ?
C4 Ir1 C3 C8 122.0(8) . . . . ?
Cl1 Ir1 C3 C8 66.5(6) . . . . ?
Cl2 Ir1 C3 C8 -23.5(6) . . . . ?
C4 C3 C2 C1 -0.4(6) . . . . ?
C8 C3 C2 C1 -176.5(5) . . . . ?
Ir1 C3 C2 C1 61.1(3) . . . . ?
C4 C3 C2 C7 175.2(5) . . . . ?
C8 C3 C2 C7 -0.9(8) . . . . ?
Ir1 C3 C2 C7 -123.3(5) . . . . ?
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C4 C3 C2 Ir1 -61.5(3) . . . . ?
C8 C3 C2 Ir1 122.4(5) . . . . ?
C1 Ir1 C2 C3 117.9(4) . . . . ?
C5 Ir1 C2 C3 80.6(3) . . . . ?
N1 Ir1 C2 C3 175.6(3) . . . . ?
C4 Ir1 C2 C3 37.6(3) . . . . ?
Cl1 Ir1 C2 C3 12.9(5) . . . . ?
Cl2 Ir1 C2 C3 -88.8(3) . . . . ?
C5 Ir1 C2 C1 -37.4(3) . . . . ?
N1 Ir1 C2 C1 57.6(3) . . . . ?
C3 Ir1 C2 C1 -117.9(4) . . . . ?
C4 Ir1 C2 C1 -80.3(3) . . . . ?
Cl1 Ir1 C2 C1 -105.0(4) . . . . ?
Cl2 Ir1 C2 C1 153.3(3) . . . . ?
C1 Ir1 C2 C7 -122.5(7) . . . . ?
C5 Ir1 C2 C7 -159.9(6) . . . . ?
N1 Ir1 C2 C7 -64.9(6) . . . . ?
C3 Ir1 C2 C7 119.6(7) . . . . ?
C4 Ir1 C2 C7 157.1(6) . . . . ?
Cl1 Ir1 C2 C7 132.5(5) . . . . ?
Cl2 Ir1 C2 C7 30.8(5) . . . . ?
C11 C12 C13 C14 -1.8(7) . . . . ?
C16 C12 C13 C14 178.9(5) . . . . ?
C12 C13 C14 C15 1.0(8) . . . . ?
C2 C3 C4 C5 1.9(6) . . . . ?
C8 C3 C4 C5 177.9(5) . . . . ?
Ir1 C3 C4 C5 -59.0(3) . . . . ?
C2 C3 C4 C9 -177.5(5) . . . . ?
C8 C3 C4 C9 -1.5(9) . . . . ?
Ir1 C3 C4 C9 121.6(6) . . . . ?
C2 C3 C4 Ir1 60.9(3) . . . . ?
C8 C3 C4 Ir1 -123.1(5) . . . . ?
C1 Ir1 C4 C5 38.8(3) . . . . ?
C2 Ir1 C4 C5 82.0(3) . . . . ?
N1 Ir1 C4 C5 -16.7(5) . . . . ?
C3 Ir1 C4 C5 119.0(5) . . . . ?
Cl1 Ir1 C4 C5 -107.7(3) . . . . ?
Cl2 Ir1 C4 C5 163.3(2) . . . . ?
C1 Ir1 C4 C3 -80.3(3) . . . . ?
C5 Ir1 C4 C3 -119.0(5) . . . . ?
C2 Ir1 C4 C3 -37.0(3) . . . . ?
N1 Ir1 C4 C3 -135.7(3) . . . . ?
Cl1 Ir1 C4 C3 133.3(3) . . . . ?
Cl2 Ir1 C4 C3 44.3(4) . . . . ?
C1 Ir1 C4 C9 158.0(7) . . . . ?
C5 Ir1 C4 C9 119.2(7) . . . . ?
C2 Ir1 C4 C9 -158.8(7) . . . . ?
N1 Ir1 C4 C9 102.5(6) . . . . ?
C3 Ir1 C4 C9 -121.8(7) . . . . ?
Cl1 Ir1 C4 C9 11.5(6) . . . . ?
Cl2 Ir1 C4 C9 -77.5(6) . . . . ?
C11 N1 C15 C14 -1.8(7) . . . . ?
Ir1 N1 C15 C14 162.0(4) . . . . ?
C13 C14 C15 N1 0.9(8) . . . . ?
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C3 C2 C1 C5 -1.2(5) . . . . ?
C7 C2 C1 C5 -176.7(5) . . . . ?
Ir1 C2 C1 C5 60.2(3) . . . . ?
C3 C2 C1 C6 178.5(5) . . . . ?
C7 C2 C1 C6 3.1(8) . . . . ?
Ir1 C2 C1 C6 -120.0(5) . . . . ?
C3 C2 C1 Ir1 -61.5(3) . . . . ?
C7 C2 C1 Ir1 123.1(5) . . . . ?
C5 Ir1 C1 C2 119.1(4) . . . . ?
N1 Ir1 C1 C2 -129.8(3) . . . . ?
C3 Ir1 C1 C2 37.4(3) . . . . ?
C4 Ir1 C1 C2 80.7(3) . . . . ?
Cl1 Ir1 C1 C2 141.8(3) . . . . ?
Cl2 Ir1 C1 C2 -36.6(4) . . . . ?
C2 Ir1 C1 C5 -119.1(4) . . . . ?
N1 Ir1 C1 C5 111.1(3) . . . . ?
C3 Ir1 C1 C5 -81.7(3) . . . . ?
C4 Ir1 C1 C5 -38.4(3) . . . . ?
Cl1 Ir1 C1 C5 22.7(4) . . . . ?
Cl2 Ir1 C1 C5 -155.7(2) . . . . ?
C5 Ir1 C1 C6 -119.5(6) . . . . ?
C2 Ir1 C1 C6 121.4(6) . . . . ?
N1 Ir1 C1 C6 -8.4(5) . . . . ?
C3 Ir1 C1 C6 158.8(5) . . . . ?
C4 Ir1 C1 C6 -157.9(5) . . . . ?
Cl1 Ir1 C1 C6 -96.8(5) . . . . ?
Cl2 Ir1 C1 C6 84.8(5) . . . . ?
C3 C4 C5 C1 -2.6(5) . . . . ?
C9 C4 C5 C1 176.8(5) . . . . ?
Ir1 C4 C5 C1 -61.8(3) . . . . ?
C3 C4 C5 C10 -176.6(5) . . . . ?
C9 C4 C5 C10 2.9(9) . . . . ?
Ir1 C4 C5 C10 124.3(5) . . . . ?
C3 C4 C5 Ir1 59.2(3) . . . . ?
C9 C4 C5 Ir1 -121.4(5) . . . . ?
C2 C1 C5 C4 2.4(5) . . . . ?
C6 C1 C5 C4 -177.4(5) . . . . ?
Ir1 C1 C5 C4 62.8(3) . . . . ?
C2 C1 C5 C10 176.5(5) . . . . ?
C6 C1 C5 C10 -3.3(8) . . . . ?
Ir1 C1 C5 C10 -123.1(5) . . . . ?
C2 C1 C5 Ir1 -60.4(3) . . . . ?
C6 C1 C5 Ir1 119.8(5) . . . . ?
C1 Ir1 C5 C4 -116.6(4) . . . . ?
C2 Ir1 C5 C4 -79.5(3) . . . . ?
N1 Ir1 C5 C4 169.5(3) . . . . ?
C3 Ir1 C5 C4 -37.2(3) . . . . ?
Cl1 Ir1 C5 C4 77.9(3) . . . . ?
Cl2 Ir1 C5 C4 -45.4(6) . . . . ?
C2 Ir1 C5 C1 37.0(3) . . . . ?
N1 Ir1 C5 C1 -73.9(3) . . . . ?
C3 Ir1 C5 C1 79.4(3) . . . . ?
C4 Ir1 C5 C1 116.6(4) . . . . ?
Cl1 Ir1 C5 C1 -165.5(2) . . . . ?
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Cl2 Ir1 C5 C1 71.2(6) . . . . ?
C1 Ir1 C5 C10 120.0(7) . . . . ?
C2 Ir1 C5 C10 157.0(6) . . . . ?
N1 Ir1 C5 C10 46.0(6) . . . . ?
C3 Ir1 C5 C10 -160.7(6) . . . . ?
C4 Ir1 C5 C10 -123.5(7) . . . . ?
Cl1 Ir1 C5 C10 -45.6(6) . . . . ?
Cl2 Ir1 C5 C10 -168.8(4) . . . . ?

_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              26.37
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    1.257
_refine_diff_density_min   -1.205
_refine_diff_density_rms    0.126
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