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data_p21-ir

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C16 H21 Cl2 Ir N2 O'
_chemical_formula_weight          520.45

loop_
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 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
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 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cl'  'Cl'   0.1484   0.1585
 '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'

_symmetry_cell_setting            Monoclinic
_symmetry_space_group_name_H-M    P21
_symmetry_space_group_name_Hall   'P 2yb'

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

_cell_length_a                    7.5416(15)
_cell_length_b                    13.907(3)
_cell_length_c                    9.0916(18)
_cell_angle_alpha                 90.00
_cell_angle_beta                  113.68(3)
_cell_angle_gamma                 90.00
_cell_volume                      873.3(3)
_cell_formula_units_Z             2
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     16432
_cell_measurement_theta_min       1.45
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```
_cell_measurement_theta_max       24.85

_exptl_crystal_description        Block
_exptl_crystal_colour             Yellow
_exptl_crystal_size_max           0.3549
_exptl_crystal_size_mid           0.2689
_exptl_crystal_size_min           0.1488
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.979
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              500
_exptl_absorpt_coefficient_mu     7.953
_exptl_absorpt_correction_type    Numerical
_exptl_absorpt_correction_T_min   0.6041
_exptl_absorpt_correction_T_max   0.8627
_exptl_absorpt_process_details    "STOE & Cie GmbH, 2004"

_exptl_special_details
;
A numerical absorption correction was based on
the crystal shape that was originally derived from
the optical face indexing but later optimized
against equivalent reflections using STOE X-Shape
software  (STOE & Cie GmbH, 2004)
;

_diffrn_ambient_temperature       293(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'fine-focus sealed tube'
_diffrn_radiation_monochromator   graphite
_diffrn_measurement_device_type   ?
_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean  ?
_diffrn_reflns_number             16390
_diffrn_reflns_av_R_equivalents   0.0504
_diffrn_reflns_av_sigmaI/netI     0.0324
_diffrn_reflns_limit_h_min        -8
_diffrn_reflns_limit_h_max        8
_diffrn_reflns_limit_k_min        -16
_diffrn_reflns_limit_k_max        16
_diffrn_reflns_limit_l_min        -10
_diffrn_reflns_limit_l_max        10
_diffrn_reflns_theta_min          2.45
_diffrn_reflns_theta_max          24.84
_reflns_number_total              2998
_reflns_number_gt                 2771
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        X-Area
_computing_cell_refinement        X-Area
_computing_data_reduction         X-Red32
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
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_computing_molecular_graphics     ?
_computing_publication_material   'SHELXL-97 (Sheldrick, 1997)'

_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^)+(0.0374P)^2^+0.4538P] 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     constr
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0028(4)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_abs_structure_details
 'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    0.0(5)
_refine_ls_number_reflns          2998
_refine_ls_number_parameters      151
_refine_ls_number_restraints      1
_refine_ls_R_factor_all           0.0271
_refine_ls_R_factor_gt            0.0243
_refine_ls_wR_factor_ref          0.0584
_refine_ls_wR_factor_gt           0.0576
_refine_ls_goodness_of_fit_ref    1.044
_refine_ls_restrained_S_all       1.043
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

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 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
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 _atom_site_symmetry_multiplicity
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Ir1 Ir 0.46777(3) 0.9597(3) 0.13734(2) 0.02796(10) Uani 1 1 d . . .
Cl1 Cl 0.6910(9) 1.0818(2) 0.1460(8) 0.0522(14) Uani 1 1 d . . .
Cl2 Cl 0.7115(8) 0.8401(2) 0.1497(7) 0.0454(12) Uani 1 1 d . . .
O1 O 0.1089(12) 1.1438(8) -0.4893(9) 0.086(3) Uani 1 1 d . . .
N2 N 0.3254(2) 1.0942(3) -0.1821(2) 0.046(2) Uani 1 1 d . . .
H2A H 0.2819 1.1435 -0.2431 0.056 Uiso 1 1 calc R . .
H2B H 0.4010 1.1018 -0.0826 0.056 Uiso 1 1 calc R . .
C1 C 0.1810(2) 0.9626(3) 0.1258(2) 0.0419(18) Uani 1 1 d R . .
C2 C 0.2775(2) 0.8806(3) 0.2141(2) 0.057(5) Uani 1 1 d R . .
C3 C 0.4366(2) 0.9126(3) 0.3522(2) 0.041(4) Uani 1 1 d R . .
C4 C 0.4384(2) 1.0144(3) 0.3493(2) 0.039(4) Uani 1 1 d R . .
C5 C 0.2805(2) 1.0453(3) 0.2094(2) 0.030(3) Uani 1 1 d R . .
C6 C 0.0039(2) 0.9619(3) -0.0296(2) 0.0612(19) Uani 1 1 d R . .
H6A H 0.0163 1.0106 -0.0998 0.092 Uiso 1 1 calc R . .
H6B H -0.1087 0.9747 -0.0084 0.092 Uiso 1 1 calc R . .
H6C H -0.0089 0.9001 -0.0798 0.092 Uiso 1 1 calc R . .
C7 C 0.2209(2) 0.7775(3) 0.1690(2) 0.052(4) Uani 1 1 d R . .
H7A H 0.1210 0.7748 0.0625 0.078 Uiso 1 1 calc R . .
H7B H 0.1740 0.7499 0.2434 0.078 Uiso 1 1 calc R . .
H7C H 0.3317 0.7420 0.1725 0.078 Uiso 1 1 calc R . .
C8 C 0.5788(2) 0.8496(3) 0.4798(2) 0.050(4) Uani 1 1 d R . .
H8A H 0.7069 0.8754 0.5116 0.075 Uiso 1 1 calc R . .
H8B H 0.5746 0.7858 0.4380 0.075 Uiso 1 1 calc R . .
H8C H 0.5455 0.8473 0.5712 0.075 Uiso 1 1 calc R . .
C9 C 0.5829(2) 1.0785(3) 0.4732(2) 0.078(6) Uani 1 1 d R . .
H9A H 0.6307 1.1254 0.4207 0.116 Uiso 1 1 calc R . .
H9B H 0.6887 1.0404 0.5444 0.116 Uiso 1 1 calc R . .
H9C H 0.5214 1.1106 0.5337 0.116 Uiso 1 1 calc R . .
C10 C 0.2276(2) 1.1480(3) 0.1584(2) 0.094(7) Uani 1 1 d R . .
H10A H 0.3431 1.1843 0.1781 0.141 Uiso 1 1 calc R . .
H10B H 0.1604 1.1752 0.2186 0.141 Uiso 1 1 calc R . .
H10C H 0.1454 1.1500 0.0459 0.141 Uiso 1 1 calc R . .
N1 N 0.3576(2) 0.9374(3) -0.1256(2) 0.0325(18) Uani 1 1 d R . .
C11 C 0.3185(2) 0.8415(3) -0.1679(2) 0.065(5) Uani 1 1 d R . .
H11 H 0.3725 0.7937 -0.0913 0.077 Uiso 1 1 calc R . .
C12 C 0.1991(2) 0.8169(3) -0.3242(2) 0.056(2) Uani 1 1 d R . .
H12 H 0.1728 0.7526 -0.3525 0.067 Uiso 1 1 calc R . .
C13 C 0.1187(2) 0.8882(3) -0.4383(2) 0.155(13) Uani 1 1 d R . .
H13 H 0.0385 0.8717 -0.5432 0.186 Uiso 1 1 calc R . .
C14 C 0.1577(2) 0.9840(3) -0.3960(2) 0.090(9) Uani 1 1 d R . .
C15 C 0.2772(2) 1.0086(3) -0.2397(2) 0.0396(17) Uani 1 1 d R . .
C16 C 0.0828(2) 1.0540(3) -0.5024(2) 0.085(4) Uani 1 1 d R . .
H16 H -0.0030 1.0335 -0.6033 0.102 Uiso 1 1 calc R . .

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 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
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 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
Ir1 0.02885(12) 0.02655(13) 0.02612(12) -0.0015(4) 0.00858(8) -0.0008(4)
Cl1 0.047(2) 0.046(3) 0.068(3) 0.001(2) 0.027(2) -0.0138(18)
Cl2 0.0412(19) 0.040(2) 0.058(3) 0.0178(19) 0.0224(17) 0.0167(16)
O1 0.078(5) 0.094(7) 0.062(4) 0.034(4) 0.001(4) 0.009(5)
N2 0.067(7) 0.031(4) 0.034(5) -0.008(3) 0.013(5) -0.007(4)
C1 0.032(3) 0.058(5) 0.039(3) 0.030(8) 0.018(3) 0.025(9)
C2 0.050(10) 0.050(9) 0.094(13) 0.026(8) 0.052(10) 0.000(7)
C3 0.048(11) 0.039(7) 0.033(9) 0.012(6) 0.012(8) 0.006(7)
C4 0.040(10) 0.050(8) 0.042(10) 0.004(7) 0.032(9) 0.010(7)
C5 0.045(8) 0.026(7) 0.017(5) 0.014(5) 0.011(5) 0.003(5)
C6 0.034(3) 0.101(6) 0.043(3) -0.001(19) 0.010(3) 0.00(2)
C7 0.069(9) 0.055(9) 0.061(8) -0.008(7) 0.056(8) -0.017(7)
C8 0.052(9) 0.065(9) 0.042(9) 0.019(7) 0.029(8) 0.033(8)
C9 0.094(14) 0.069(11) 0.055(11) -0.031(9) 0.014(10) 0.012(10)
C10 0.104(15) 0.030(8) 0.115(14) 0.006(9) 0.009(11) 0.030(9)
N1 0.037(3) 0.019(6) 0.044(3) 0.015(2) 0.019(2) 0.010(2)
C11 0.037(6) 0.122(13) 0.030(7) -0.049(8) 0.009(6) -0.006(7)
C12 0.060(5) 0.055(6) 0.054(5) -0.015(4) 0.023(5) -0.005(4)
C13 0.138(17) 0.23(3) 0.119(14) 0.097(18) 0.075(12) 0.13(2)
C14 0.027(4) 0.20(3) 0.042(4) -0.041(9) 0.016(3) -0.029(8)
C15 0.042(4) 0.042(4) 0.031(4) -0.001(3) 0.010(3) 0.001(4)
C16 0.088(10) 0.088(10) 0.108(11) -0.046(9) 0.068(8) -0.020(8)

_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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 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
Ir1 C1 2.1228(16) . ?
Ir1 C2 2.135(2) . ?
Ir1 C5 2.141(2) . ?
Ir1 C3 2.1611(19) . ?
Ir1 C4 2.165(2) . ?
Ir1 N1 2.2153(19) . ?
Ir1 Cl1 2.370(6) . ?
Ir1 Cl2 2.448(6) . ?
```

```
O1 C16 1.262(11) . ?
N2 C15 1.2920 . ?
N2 H2A 0.8600 . ?
N2 H2B 0.8600 . ?
C1 C2 1.4159 . ?
C1 C5 1.4159 . ?
C1 C6 1.5051 . ?
C2 C3 1.4159 . ?
C2 C7 1.5050 . ?
C3 C4 1.4159 . ?
C3 C8 1.5051 . ?
C4 C5 1.4159 . ?
C4 C9 1.5051 . ?
C5 C10 1.5050 . ?
C6 H6A 0.9600 . ?
C6 H6B 0.9600 . ?
C6 H6C 0.9600 . ?
C7 H7A 0.9600 . ?
C7 H7B 0.9600 . ?
C7 H7C 0.9600 . ?
C8 H8A 0.9600 . ?
C8 H8B 0.9600 . ?
C8 H8C 0.9600 . ?
C9 H9A 0.9600 . ?
C9 H9B 0.9600 . ?
C9 H9C 0.9600 . ?
C10 H10A 0.9600 . ?
C10 H10B 0.9600 . ?
C10 H10C 0.9600 . ?
N1 C11 1.3857 . ?
N1 C15 1.3857 . ?
C11 C12 1.3857 . ?
C11 H11 0.9300 . ?
C12 C13 1.3857 . ?
C12 H12 0.9300 . ?
C13 C14 1.3857 . ?
C13 H13 0.9300 . ?
C14 C16 1.3282 . ?
C14 C15 1.3857 . ?
C16 H16 0.9300 . ?

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 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_3
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C1 Ir1 C2 38.8 . . ?
C1 Ir1 C5 38.8 . . ?
C2 Ir1 C5 64.8 . . ?
C1 Ir1 C3 64.6 . . ?
C2 Ir1 C3 38.5 . . ?
```

```
C5 Ir1 C3 64.3 . . ?
C1 Ir1 C4 64.6 . . ?
C2 Ir1 C4 64.4 . . ?
C5 Ir1 C4 38.4 . . ?
C3 Ir1 C4 38.2 . . ?
C1 Ir1 N1 90.93(8) . . ?
C2 Ir1 N1 105.70(11) . . ?
C5 Ir1 N1 113.61(9) . . ?
C3 Ir1 N1 143.47(14) . . ?
C4 Ir1 N1 151.90(10) . . ?
C1 Ir1 Cl1 133.16(18) . . ?
C2 Ir1 Cl1 156.88(17) . . ?
C5 Ir1 Cl1 97.97(18) . . ?
C3 Ir1 Cl1 121.38(18) . . ?
C4 Ir1 Cl1 92.51(18) . . ?
N1 Ir1 Cl1 95.15(18) . . ?
C1 Ir1 Cl2 138.27(17) . . ?
C2 Ir1 Cl2 103.04(15) . . ?
C5 Ir1 Cl2 159.92(14) . . ?
C3 Ir1 Cl2 96.03(15) . . ?
C4 Ir1 Cl2 122.79(15) . . ?
N1 Ir1 Cl2 84.46(16) . . ?
Cl1 Ir1 Cl2 88.57(9) . . ?
C15 N2 H2A 120.0 . . ?
C15 N2 H2B 120.0 . . ?
H2A N2 H2B 120.0 . . ?
C2 C1 C5 108.0 . . ?
C2 C1 C6 126.0 . . ?
C5 C1 C6 126.0 . . ?
C2 C1 Ir1 71.06(8) . . ?
C5 C1 Ir1 71.30(8) . . ?
C6 C1 Ir1 123.3 . . ?
C3 C2 C1 108.0 . . ?
C3 C2 C7 126.0 . . ?
C1 C2 C7 126.0 . . ?
C3 C2 Ir1 71.75(5) . . ?
C1 C2 Ir1 70.10(7) . . ?
C7 C2 Ir1 123.78(8) . . ?
C2 C3 C4 108.0 . . ?
C2 C3 C8 126.0 . . ?
C4 C3 C8 126.0 . . ?
C2 C3 Ir1 69.78(6) . . ?
C4 C3 Ir1 71.03(8) . . ?
C8 C3 Ir1 124.79(6) . . ?
C5 C4 C3 108.0 . . ?
C5 C4 C9 126.0 . . ?
C3 C4 C9 126.0 . . ?
C5 C4 Ir1 69.90(6) . . ?
C3 C4 Ir1 70.76(8) . . ?
C9 C4 Ir1 124.93(6) . . ?
C4 C5 C1 108.0 . . ?
C4 C5 C10 126.0 . . ?
C1 C5 C10 126.0 . . ?
C4 C5 Ir1 71.7 . . ?
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```
C1 C5 Ir1 69.91(7) . . ?
C10 C5 Ir1 124.00(7) . . ?
C1 C6 H6A 109.5 . . ?
C1 C6 H6B 109.5 . . ?
H6A C6 H6B 109.5 . . ?
C1 C6 H6C 109.5 . . ?
H6A C6 H6C 109.5 . . ?
H6B C6 H6C 109.5 . . ?
C2 C7 H7A 109.5 . . ?
C2 C7 H7B 109.5 . . ?
H7A C7 H7B 109.5 . . ?
C2 C7 H7C 109.5 . . ?
H7A C7 H7C 109.5 . . ?
H7B C7 H7C 109.5 . . ?
C3 C8 H8A 109.5 . . ?
C3 C8 H8B 109.5 . . ?
H8A C8 H8B 109.5 . . ?
C3 C8 H8C 109.5 . . ?
H8A C8 H8C 109.5 . . ?
H8B C8 H8C 109.5 . . ?
C4 C9 H9A 109.5 . . ?
C4 C9 H9B 109.5 . . ?
H9A C9 H9B 109.5 . . ?
C4 C9 H9C 109.5 . . ?
H9A C9 H9C 109.5 . . ?
H9B C9 H9C 109.5 . . ?
C5 C10 H10A 109.5 . . ?
C5 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
C5 C10 H10C 109.5 . . ?
H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
C11 N1 C15 120.0 . . ?
C11 N1 Ir1 112.32(8) . . ?
C15 N1 Ir1 124.71(8) . . ?
N1 C11 C12 120.0 . . ?
N1 C11 H11 120.0 . . ?
C12 C11 H11 120.0 . . ?
C13 C12 C11 120.0 . . ?
C13 C12 H12 120.0 . . ?
C11 C12 H12 120.0 . . ?
C12 C13 C14 120.0 . . ?
C12 C13 H13 120.0 . . ?
C14 C13 H13 120.0 . . ?
C16 C14 C15 118.5 . . ?
C16 C14 C13 121.5 . . ?
C15 C14 C13 120.0 . . ?
N2 C15 C14 127.2 . . ?
N2 C15 N1 112.8 . . ?
C14 C15 N1 120.0 . . ?
O1 C16 C14 130.7(3) . . ?
O1 C16 H16 114.7 . . ?
C14 C16 H16 114.7 . . ?
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C5 Ir1 C1 C2 -117.5 . . . . ?
C3 Ir1 C1 C2 -37.5 . . . . ?
C4 Ir1 C1 C2 -80.0 . . . . ?
N1 Ir1 C1 C2 114.28(10) . . . . ?
Cl1 Ir1 C1 C2 -147.8(2) . . . . ?
Cl2 Ir1 C1 C2 31.6(2) . . . . ?
C2 Ir1 C1 C5 117.5 . . . . ?
C3 Ir1 C1 C5 79.9 . . . . ?
C4 Ir1 C1 C5 37.4 . . . . ?
N1 Ir1 C1 C5 -128.26(10) . . . . ?
Cl1 Ir1 C1 C5 -30.3(2) . . . . ?
Cl2 Ir1 C1 C5 149.0(2) . . . . ?
C2 Ir1 C1 C6 -121.2 . . . . ?
C5 Ir1 C1 C6 121.3 . . . . ?
C3 Ir1 C1 C6 -158.7 . . . . ?
C4 Ir1 C1 C6 158.8 . . . . ?
N1 Ir1 C1 C6 -6.92(14) . . . . ?
Cl1 Ir1 C1 C6 91.0(2) . . . . ?
Cl2 Ir1 C1 C6 -89.6(2) . . . . ?
C5 C1 C2 C3 0.0 . . . . ?
C6 C1 C2 C3 180.0 . . . . ?
Ir1 C1 C2 C3 62.10(7) . . . . ?
C5 C1 C2 C7 180.0 . . . . ?
C6 C1 C2 C7 0.0 . . . . ?
Ir1 C1 C2 C7 -117.89(7) . . . . ?
C5 C1 C2 Ir1 -62.10(7) . . . . ?
C6 C1 C2 Ir1 117.90(7) . . . . ?
C1 Ir1 C2 C3 -117.7 . . . . ?
C5 Ir1 C2 C3 -79.8 . . . . ?
C4 Ir1 C2 C3 -37.1 . . . . ?
N1 Ir1 C2 C3 171.05(12) . . . . ?
Cl1 Ir1 C2 C3 -35.3(4) . . . . ?
Cl2 Ir1 C2 C3 83.22(15) . . . . ?
C5 Ir1 C2 C1 37.9 . . . . ?
C3 Ir1 C2 C1 117.7 . . . . ?
C4 Ir1 C2 C1 80.6 . . . . ?
N1 Ir1 C2 C1 -71.21(8) . . . . ?
Cl1 Ir1 C2 C1 82.4(4) . . . . ?
Cl2 Ir1 C2 C1 -159.04(15) . . . . ?
C1 Ir1 C2 C7 120.7 . . . . ?
C5 Ir1 C2 C7 158.6 . . . . ?
C3 Ir1 C2 C7 -121.6 . . . . ?
C4 Ir1 C2 C7 -158.7 . . . . ?
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N1 Ir1 C2 C7 49.45(12) . . . . ?
Cl1 Ir1 C2 C7 -156.9(4) . . . . ?
Cl2 Ir1 C2 C7 -38.38(16) . . . . ?
C1 C2 C3 C4 0.0 . . . . ?
C7 C2 C3 C4 180.0 . . . . ?
Ir1 C2 C3 C4 61.05(8) . . . . ?
C1 C2 C3 C8 180.0 . . . . ?
C7 C2 C3 C8 0.0 . . . . ?
Ir1 C2 C3 C8 -118.95(8) . . . . ?
C1 C2 C3 Ir1 -61.05(8) . . . . ?
C7 C2 C3 Ir1 118.95(8) . . . . ?
C1 Ir1 C3 C2 37.9 . . . . ?
C5 Ir1 C3 C2 81.1 . . . . ?
C4 Ir1 C3 C2 118.4 . . . . ?
N1 Ir1 C3 C2 -14.57(17) . . . . ?
Cl1 Ir1 C3 C2 164.6(2) . . . . ?
Cl2 Ir1 C3 C2 -103.39(16) . . . . ?
C1 Ir1 C3 C4 -80.46(6) . . . . ?
C2 Ir1 C3 C4 -118.4 . . . . ?
C5 Ir1 C3 C4 -37.3 . . . . ?
N1 Ir1 C3 C4 -132.9(2) . . . . ?
Cl1 Ir1 C3 C4 46.24(19) . . . . ?
Cl2 Ir1 C3 C4 138.25(15) . . . . ?
C1 Ir1 C3 C8 158.3 . . . . ?
C2 Ir1 C3 C8 120.5 . . . . ?
C5 Ir1 C3 C8 -158.5 . . . . ?
C4 Ir1 C3 C8 -121.20(5) . . . . ?
N1 Ir1 C3 C8 105.88(16) . . . . ?
Cl1 Ir1 C3 C8 -75.0(2) . . . . ?
Cl2 Ir1 C3 C8 17.06(16) . . . . ?
C2 C3 C4 C5 0.0 . . . . ?
C8 C3 C4 C5 180.0 . . . . ?
Ir1 C3 C4 C5 60.3 . . . . ?
C2 C3 C4 C9 180.0 . . . . ?
C8 C3 C4 C9 0.0 . . . . ?
Ir1 C3 C4 C9 -119.7 . . . . ?
C2 C3 C4 Ir1 -60.3 . . . . ?
C8 C3 C4 Ir1 119.7 . . . . ?
C1 Ir1 C4 C5 -37.8 . . . . ?
C2 Ir1 C4 C5 -81.0 . . . . ?
C3 Ir1 C4 C5 -118.4 . . . . ?
N1 Ir1 C4 C5 -6.2(3) . . . . ?
Cl1 Ir1 C4 C5 99.68(17) . . . . ?
Cl2 Ir1 C4 C5 -170.40(18) . . . . ?
C1 Ir1 C4 C3 80.63(6) . . . . ?
C2 Ir1 C4 C3 37.4 . . . . ?
C5 Ir1 C4 C3 118.4 . . . . ?
N1 Ir1 C4 C3 112.3(3) . . . . ?
Cl1 Ir1 C4 C3 -141.89(17) . . . . ?
Cl2 Ir1 C4 C3 -51.96(17) . . . . ?
C1 Ir1 C4 C9 -158.3 . . . . ?
C2 Ir1 C4 C9 158.4 . . . . ?
C5 Ir1 C4 C9 -120.5 . . . . ?
C3 Ir1 C4 C9 121.0 . . . . ?
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N1 Ir1 C4 C9 -126.7(3) . . . . ?
Cl1 Ir1 C4 C9 -20.85(17) . . . . ?
Cl2 Ir1 C4 C9 69.07(19) . . . . ?
C3 C4 C5 C1 0.0 . . . . ?
C9 C4 C5 C1 180.0 . . . . ?
Ir1 C4 C5 C1 60.80(8) . . . . ?
C3 C4 C5 C10 180.0 . . . . ?
C9 C4 C5 C10 0.0 . . . . ?
Ir1 C4 C5 C10 -119.19(8) . . . . ?
C3 C4 C5 Ir1 -60.80(8) . . . . ?
C9 C4 C5 Ir1 119.20(8) . . . . ?
C2 C1 C5 C4 0.0 . . . . ?
C6 C1 C5 C4 180.0 . . . . ?
Ir1 C1 C5 C4 -61.95(6) . . . . ?
C2 C1 C5 C10 180.0 . . . . ?
C6 C1 C5 C10 0.0 . . . . ?
Ir1 C1 C5 C10 118.05(6) . . . . ?
C2 C1 C5 Ir1 61.95(6) . . . . ?
C6 C1 C5 Ir1 -118.05(6) . . . . ?
C1 Ir1 C5 C4 117.9 . . . . ?
C2 Ir1 C5 C4 79.9 . . . . ?
C3 Ir1 C5 C4 37.1 . . . . ?
N1 Ir1 C5 C4 176.83(14) . . . . ?
Cl1 Ir1 C5 C4 -83.95(17) . . . . ?
Cl2 Ir1 C5 C4 24.1(5) . . . . ?
C2 Ir1 C5 C1 -38.0 . . . . ?
C3 Ir1 C5 C1 -80.76(6) . . . . ?
C4 Ir1 C5 C1 -117.9 . . . . ?
N1 Ir1 C5 C1 58.96(10) . . . . ?
Cl1 Ir1 C5 C1 158.18(17) . . . . ?
Cl2 Ir1 C5 C1 -93.8(5) . . . . ?
C1 Ir1 C5 C10 -120.5 . . . . ?
C2 Ir1 C5 C10 -158.5 . . . . ?
C3 Ir1 C5 C10 158.7 . . . . ?
C4 Ir1 C5 C10 121.6 . . . . ?
N1 Ir1 C5 C10 -61.58(14) . . . . ?
Cl1 Ir1 C5 C10 37.63(17) . . . . ?
Cl2 Ir1 C5 C10 145.7(5) . . . . ?
C1 Ir1 N1 C11 -83.75(9) . . . . ?
C2 Ir1 N1 C11 -47.32(10) . . . . ?
C5 Ir1 N1 C11 -116.21(12) . . . . ?
C3 Ir1 N1 C11 -38.0(2) . . . . ?
C4 Ir1 N1 C11 -112.0(3) . . . . ?
Cl1 Ir1 N1 C11 142.76(16) . . . . ?
Cl2 Ir1 N1 C11 54.70(14) . . . . ?
C1 Ir1 N1 C15 76.60(11) . . . . ?
C2 Ir1 N1 C15 113.02(11) . . . . ?
C5 Ir1 N1 C15 44.13(14) . . . . ?
C3 Ir1 N1 C15 122.4(2) . . . . ?
C4 Ir1 N1 C15 48.3(3) . . . . ?
Cl1 Ir1 N1 C15 -56.90(17) . . . . ?
Cl2 Ir1 N1 C15 -144.96(15) . . . . ?
C15 N1 C11 C12 0.0 . . . . ?
Ir1 N1 C11 C12 161.4 . . . . ?
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N1 C11 C12 C13 0.0 . . . . ?
C11 C12 C13 C14 0.0 . . . . ?
C12 C13 C14 C16 -179.9 . . . . ?
C12 C13 C14 C15 0.0 . . . . ?
C16 C14 C15 N2 0.6 . . . . ?
C13 C14 C15 N2 -179.3 . . . . ?
C16 C14 C15 N1 179.9 . . . . ?
C13 C14 C15 N1 0.0 . . . . ?
C11 N1 C15 N2 179.4 . . . . ?
Ir1 N1 C15 N2 20.46(6) . . . . ?
C11 N1 C15 C14 0.0 . . . . ?
Ir1 N1 C15 C14 -158.94(6) . . . . ?
C15 C14 C16 O1 4.2(5) . . . . ?
C13 C14 C16 O1 -175.9(5) . . . . ?

_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              24.84
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    1.310
_refine_diff_density_min   -0.757
_refine_diff_density_rms    0.123
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