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data_pbca

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_chemical_name_systematic
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;
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_chemical_formula_moiety          ?
_chemical_formula_sum
 'C15 H20 Cl2 Ir N3 O2'
_chemical_formula_weight          537.44

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 _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            Orthorhombic
_symmetry_space_group_name_H-M    Pbca
_symmetry_space_group_name_Hall   '-P 2ac 2ab'

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

_cell_length_a                    7.5125(15)
_cell_length_b                    15.018(3)
_cell_length_c                    30.912(6)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
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```
_cell_angle_gamma                  90.00
_cell_volume                       3487.6(12)
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_exptl_crystal_size_mid            ?
_exptl_crystal_size_min            ?
_exptl_crystal_density_meas        ?
_exptl_crystal_density_diffrn      2.047
_exptl_crystal_density_method      'not measured'
_exptl_crystal_F_000               2064
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_exptl_special_details
;
 ?
;

_diffrn_ambient_temperature        293(2)
_diffrn_radiation_wavelength       0.71073
_diffrn_radiation_type             MoK\a
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_diffrn_reflns_limit_k_max         16
_diffrn_reflns_limit_l_min         -38
_diffrn_reflns_limit_l_max         34
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_computing_cell_refinement         ?
_computing_data_reduction          ?
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_computing_molecular_graphics     ?
_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.
;

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_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0000P)^2^+29.6838P] 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      none
_refine_ls_extinction_coef        ?
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_refine_ls_number_restraints      0
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_refine_ls_goodness_of_fit_ref    1.362
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Cl1 Cl 0.3804(3) 0.68121(14) 0.38398(7) 0.0374(5) Uani 1 1 d . . .
Cl2 Cl 0.3814(3) 0.88799(14) 0.42242(7) 0.0390(5) Uani 1 1 d . . .
O1 O 0.0465(16) 1.0798(5) 0.2845(3) 0.098(3) Uani 1 1 d . . .
O2 O 0.0101(17) 1.0268(6) 0.2218(3) 0.111(4) Uani 1 1 d . . .
N1 N 0.1731(9) 0.8295(4) 0.3319(2) 0.0288(15) Uani 1 1 d . . .
N2 N 0.1579(11) 0.9781(5) 0.3485(2) 0.045(2) Uani 1 1 d . . .
H2A H 0.1849 0.9641 0.3747 0.054 Uiso 1 1 calc R . .
H2B H 0.1404 1.0329 0.3418 0.054 Uiso 1 1 calc R . .
N3 N 0.0495(14) 1.0184(6) 0.2596(3) 0.060(2) Uani 1 1 d . . .
C1 C -0.1345(10) 0.7965(6) 0.3951(2) 0.0292(17) Uani 1 1 d . . .
C2 C -0.0834(11) 0.7060(6) 0.4005(3) 0.0348(19) Uani 1 1 d . . .
C3 C 0.0073(11) 0.7000(5) 0.4422(3) 0.0326(19) Uani 1 1 d . . .
C4 C 0.0147(10) 0.7863(6) 0.4604(2) 0.0292(17) Uani 1 1 d . . .
C5 C -0.0720(11) 0.8481(6) 0.4312(3) 0.0309(18) Uani 1 1 d . . .
C6 C -0.2394(13) 0.8316(7) 0.3572(3) 0.049(3) Uani 1 1 d . . .
H6A H -0.2196 0.8945 0.3544 0.074 Uiso 1 1 calc R . .
H6B H -0.3638 0.8206 0.3618 0.074 Uiso 1 1 calc R . .
H6C H -0.2016 0.8020 0.3312 0.074 Uiso 1 1 calc R . .
C7 C -0.1319(14) 0.6285(6) 0.3716(3) 0.051(3) Uani 1 1 d . . .
H7A H -0.0453 0.5819 0.3750 0.077 Uiso 1 1 calc R . .
H7B H -0.1336 0.6478 0.3420 0.077 Uiso 1 1 calc R . .
H7C H -0.2474 0.6064 0.3795 0.077 Uiso 1 1 calc R . .
C8 C 0.0757(14) 0.6167(6) 0.4628(3) 0.054(3) Uani 1 1 d . . .
H8A H 0.1073 0.5746 0.4407 0.081 Uiso 1 1 calc R . .
H8B H -0.0150 0.5916 0.4809 0.081 Uiso 1 1 calc R . .
H8C H 0.1787 0.6304 0.4799 0.081 Uiso 1 1 calc R . .
C9 C 0.0894(13) 0.8087(7) 0.5034(3) 0.048(3) Uani 1 1 d . . .
H9A H 0.1473 0.8656 0.5020 0.072 Uiso 1 1 calc R . .
H9B H 0.1741 0.7641 0.5118 0.072 Uiso 1 1 calc R . .
H9C H -0.0050 0.8110 0.5243 0.072 Uiso 1 1 calc R . .
C10 C -0.1057(14) 0.9446(6) 0.4392(3) 0.048(3) Uani 1 1 d . . .
H10A H -0.1280 0.9740 0.4121 0.071 Uiso 1 1 calc R . .
H10B H -0.0033 0.9708 0.4528 0.071 Uiso 1 1 calc R . .
H10C H -0.2073 0.9512 0.4577 0.071 Uiso 1 1 calc R . .
C11 C 0.1432(11) 0.9150(5) 0.3186(2) 0.0284(18) Uani 1 1 d . . .
C12 C 0.0933(12) 0.9295(6) 0.2748(3) 0.039(2) Uani 1 1 d . . .
C13 C 0.0809(12) 0.8610(6) 0.2460(3) 0.041(2) Uani 1 1 d . . .
H13 H 0.0463 0.8718 0.2176 0.050 Uiso 1 1 calc R . .
C14 C 0.1196(12) 0.7762(6) 0.2593(3) 0.041(2) Uani 1 1 d . . .
H14 H 0.1152 0.7284 0.2402 0.049 Uiso 1 1 calc R . .
C15 C 0.1656(12) 0.7649(6) 0.3023(3) 0.041(2) Uani 1 1 d . . .
H15 H 0.1936 0.7075 0.3113 0.049 Uiso 1 1 calc R . .

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 _atom_site_aniso_U_13
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Ir1 0.02855(16) 0.01836(15) 0.02515(16) -0.00226(14) 0.00281(12) -
0.00081(12)
Cl1 0.0335(11) 0.0286(11) 0.0501(13) -0.0075(9) 0.0038(9) 0.0069(9)
Cl2 0.0397(12) 0.0319(11) 0.0453(13) -0.0077(10) -0.0042(10) -0.0096(10)
O1 0.174(10) 0.044(5) 0.075(6) 0.005(5) -0.042(7) 0.015(6)
O2 0.214(12) 0.076(6) 0.042(5) 0.023(4) -0.033(7) -0.011(7)
N1 0.036(4) 0.027(4) 0.023(3) 0.001(3) 0.004(3) -0.003(3)
N2 0.077(6) 0.022(4) 0.037(4) -0.001(3) -0.003(4) 0.001(4)
N3 0.089(7) 0.049(5) 0.040(5) 0.012(4) -0.011(5) -0.008(5)
C1 0.022(4) 0.041(5) 0.025(4) 0.001(4) 0.005(3) -0.005(4)
C2 0.036(4) 0.033(5) 0.036(4) 0.007(4) 0.009(4) -0.015(4)
C3 0.034(4) 0.026(4) 0.038(5) 0.006(4) 0.011(4) 0.003(4)
C4 0.033(4) 0.033(4) 0.022(4) -0.002(3) 0.004(3) 0.007(4)
C5 0.030(4) 0.033(5) 0.029(4) -0.002(4) 0.006(3) 0.003(4)
C6 0.037(5) 0.076(7) 0.034(5) 0.011(5) -0.003(4) 0.001(5)
C7 0.056(6) 0.043(6) 0.054(6) -0.018(5) 0.015(5) -0.021(5)
C8 0.063(7) 0.039(6) 0.060(7) 0.018(5) 0.017(5) 0.016(5)
C9 0.055(6) 0.061(7) 0.028(5) -0.004(4) -0.005(4) 0.012(5)
C10 0.064(7) 0.032(5) 0.046(6) -0.008(4) 0.014(5) 0.012(5)
C11 0.036(4) 0.023(4) 0.026(4) 0.002(3) 0.003(3) -0.006(4)
C12 0.043(5) 0.039(5) 0.035(5) 0.009(4) -0.001(4) -0.007(4)
C13 0.050(5) 0.053(6) 0.021(4) -0.001(4) 0.005(4) -0.004(5)
C14 0.059(6) 0.040(5) 0.025(4) -0.011(4) 0.005(4) -0.008(5)
C15 0.052(6) 0.025(5) 0.044(5) -0.010(4) 0.015(4) -0.005(4)

_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
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Ir1 C1 2.143(7) . ?
Ir1 C5 2.146(8) . ?
Ir1 C4 2.153(7) . ?
Ir1 C3 2.155(8) . ?
Ir1 N1 2.174(6) . ?
Ir1 Cl1 2.398(2) . ?
Ir1 Cl2 2.418(2) . ?
O1 N3 1.202(11) . ?
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O2 N3 1.213(10) . ?
N1 C15 1.336(10) . ?
N1 C11 1.367(10) . ?
N2 C11 1.329(10) . ?
N2 H2A 0.8600 . ?
N2 H2B 0.8600 . ?
N3 C12 1.453(12) . ?
C1 C2 1.422(12) . ?
C1 C5 1.439(11) . ?
C1 C6 1.507(11) . ?
C2 C3 1.459(12) . ?
C2 C7 1.512(12) . ?
C3 C4 1.415(11) . ?
C3 C8 1.494(12) . ?
C4 C5 1.448(11) . ?
C4 C9 1.482(11) . ?
C5 C10 1.492(11) . ?
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 . ?
C11 C12 1.421(11) . ?
C12 C13 1.363(12) . ?
C13 C14 1.368(13) . ?
C13 H13 0.9300 . ?
C14 C15 1.385(12) . ?
C14 H14 0.9300 . ?
C15 H15 0.9300 . ?

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 _geom_angle_site_symmetry_3
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C2 Ir1 C5 66.2(3) . . ?
C1 Ir1 C5 39.2(3) . . ?
C2 Ir1 C4 65.8(3) . . ?
C1 Ir1 C4 65.2(3) . . ?
C5 Ir1 C4 39.4(3) . . ?
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C2 Ir1 C3 39.8(3) . . ?
C1 Ir1 C3 65.1(3) . . ?
C5 Ir1 C3 65.5(3) . . ?
C4 Ir1 C3 38.4(3) . . ?
C2 Ir1 N1 104.8(3) . . ?
C1 Ir1 N1 90.4(3) . . ?
C5 Ir1 N1 112.4(3) . . ?
C4 Ir1 N1 151.7(3) . . ?
C3 Ir1 N1 143.9(3) . . ?
C2 Ir1 Cl1 102.6(2) . . ?
C1 Ir1 Cl1 138.8(2) . . ?
C5 Ir1 Cl1 159.0(2) . . ?
C4 Ir1 Cl1 120.4(2) . . ?
C3 Ir1 Cl1 94.3(2) . . ?
N1 Ir1 Cl1 87.24(18) . . ?
C2 Ir1 Cl2 160.3(2) . . ?
C1 Ir1 Cl2 133.9(2) . . ?
C5 Ir1 Cl2 98.8(2) . . ?
C4 Ir1 Cl2 94.5(2) . . ?
C3 Ir1 Cl2 123.5(2) . . ?
N1 Ir1 Cl2 92.58(18) . . ?
Cl1 Ir1 Cl2 87.33(8) . . ?
C15 N1 C11 117.9(7) . . ?
C15 N1 Ir1 116.0(6) . . ?
C11 N1 Ir1 123.3(5) . . ?
C11 N2 H2A 120.0 . . ?
C11 N2 H2B 120.0 . . ?
H2A N2 H2B 120.0 . . ?
O1 N3 O2 122.3(10) . . ?
O1 N3 C12 120.1(8) . . ?
O2 N3 C12 117.5(10) . . ?
C2 C1 C5 109.5(7) . . ?
C2 C1 C6 124.6(8) . . ?
C5 C1 C6 125.9(8) . . ?
C2 C1 Ir1 70.3(4) . . ?
C5 C1 Ir1 70.5(4) . . ?
C6 C1 Ir1 126.0(6) . . ?
C1 C2 C3 106.8(7) . . ?
C1 C2 C7 126.9(8) . . ?
C3 C2 C7 125.9(8) . . ?
C1 C2 Ir1 70.9(4) . . ?
C3 C2 Ir1 70.9(5) . . ?
C7 C2 Ir1 128.6(6) . . ?
C4 C3 C2 108.2(7) . . ?
C4 C3 C8 125.7(8) . . ?
C2 C3 C8 126.0(8) . . ?
C4 C3 Ir1 70.7(4) . . ?
C2 C3 Ir1 69.4(4) . . ?
C8 C3 Ir1 127.0(6) . . ?
C3 C4 C5 108.7(7) . . ?
C3 C4 C9 125.5(8) . . ?
C5 C4 C9 125.7(8) . . ?
C3 C4 Ir1 70.9(4) . . ?
C5 C4 Ir1 70.1(4) . . ?
```

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C9 C4 Ir1 127.7(6) . . ?
C1 C5 C4 106.6(7) . . ?
C1 C5 C10 126.5(8) . . ?
C4 C5 C10 126.6(8) . . ?
C1 C5 Ir1 70.3(4) . . ?
C4 C5 Ir1 70.6(4) . . ?
C10 C5 Ir1 128.4(6) . . ?
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 . . ?
N2 C11 N1 116.5(7) . . ?
N2 C11 C12 125.2(8) . . ?
N1 C11 C12 118.3(7) . . ?
C13 C12 C11 121.6(8) . . ?
C13 C12 N3 117.8(8) . . ?
C11 C12 N3 120.6(8) . . ?
C12 C13 C14 119.5(8) . . ?
C12 C13 H13 120.2 . . ?
C14 C13 H13 120.2 . . ?
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C13 C14 H14 121.5 . . ?
C15 C14 H14 121.5 . . ?
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N1 C15 H15 117.3 . . ?
C14 C15 H15 117.3 . . ?

loop_
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C4 Ir1 N1 C15 -117.3(8) . . . . ?
C3 Ir1 N1 C15 -42.3(9) . . . . ?
Cl1 Ir1 N1 C15 51.2(6) . . . . ?
Cl2 Ir1 N1 C15 138.4(6) . . . . ?
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C4 Ir1 N1 C11 43.3(10) . . . . ?
C3 Ir1 N1 C11 118.2(7) . . . . ?
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Cl2 Ir1 N1 C11 -61.1(6) . . . . ?
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C4 Ir1 C1 C2 -81.6(5) . . . . ?
C3 Ir1 C1 C2 -39.1(5) . . . . ?
N1 Ir1 C1 C2 113.4(5) . . . . ?
Cl1 Ir1 C1 C2 27.1(6) . . . . ?
Cl2 Ir1 C1 C2 -152.6(4) . . . . ?
C2 Ir1 C1 C5 120.2(7) . . . . ?
C4 Ir1 C1 C5 38.6(5) . . . . ?
C3 Ir1 C1 C5 81.1(5) . . . . ?
N1 Ir1 C1 C5 -126.4(5) . . . . ?
Cl1 Ir1 C1 C5 147.3(4) . . . . ?
Cl2 Ir1 C1 C5 -32.4(6) . . . . ?
C2 Ir1 C1 C6 -119.0(10) . . . . ?
C5 Ir1 C1 C6 120.8(10) . . . . ?
C4 Ir1 C1 C6 159.4(9) . . . . ?
C3 Ir1 C1 C6 -158.2(9) . . . . ?
N1 Ir1 C1 C6 -5.6(8) . . . . ?
Cl1 Ir1 C1 C6 -92.0(8) . . . . ?
Cl2 Ir1 C1 C6 88.4(8) . . . . ?
C5 C1 C2 C3 2.3(9) . . . . ?
C6 C1 C2 C3 -177.1(7) . . . . ?
Ir1 C1 C2 C3 62.1(5) . . . . ?
C5 C1 C2 C7 175.8(8) . . . . ?
C6 C1 C2 C7 -3.7(13) . . . . ?
Ir1 C1 C2 C7 -124.4(8) . . . . ?
C5 C1 C2 Ir1 -59.8(5) . . . . ?
C6 C1 C2 Ir1 120.7(8) . . . . ?
C5 Ir1 C2 C1 36.7(5) . . . . ?
C4 Ir1 C2 C1 79.9(5) . . . . ?
C3 Ir1 C2 C1 116.4(7) . . . . ?
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N1 Ir1 C2 C1 -71.7(5) . . . . ?
Cl1 Ir1 C2 C1 -162.1(4) . . . . ?
Cl2 Ir1 C2 C1 79.1(8) . . . . ?
C1 Ir1 C2 C3 -116.4(7) . . . . ?
C5 Ir1 C2 C3 -79.8(5) . . . . ?
C4 Ir1 C2 C3 -36.5(5) . . . . ?
N1 Ir1 C2 C3 171.9(4) . . . . ?
Cl1 Ir1 C2 C3 81.5(5) . . . . ?
Cl2 Ir1 C2 C3 -37.3(10) . . . . ?
C1 Ir1 C2 C7 122.5(10) . . . . ?
C5 Ir1 C2 C7 159.1(9) . . . . ?
C4 Ir1 C2 C7 -157.6(9) . . . . ?
C3 Ir1 C2 C7 -121.1(10) . . . . ?
N1 Ir1 C2 C7 50.8(9) . . . . ?
Cl1 Ir1 C2 C7 -39.6(9) . . . . ?
Cl2 Ir1 C2 C7 -158.4(6) . . . . ?
C1 C2 C3 C4 -1.8(9) . . . . ?
C7 C2 C3 C4 -175.3(8) . . . . ?
Ir1 C2 C3 C4 60.3(6) . . . . ?
C1 C2 C3 C8 176.4(8) . . . . ?
C7 C2 C3 C8 2.9(13) . . . . ?
Ir1 C2 C3 C8 -121.5(8) . . . . ?
C1 C2 C3 Ir1 -62.1(5) . . . . ?
C7 C2 C3 Ir1 124.3(8) . . . . ?
C2 Ir1 C3 C4 -119.0(7) . . . . ?
C1 Ir1 C3 C4 -80.8(5) . . . . ?
C5 Ir1 C3 C4 -37.5(5) . . . . ?
N1 Ir1 C3 C4 -132.4(5) . . . . ?
Cl1 Ir1 C3 C4 136.4(4) . . . . ?
Cl2 Ir1 C3 C4 46.7(5) . . . . ?
C1 Ir1 C3 C2 38.2(5) . . . . ?
C5 Ir1 C3 C2 81.6(5) . . . . ?
C4 Ir1 C3 C2 119.0(7) . . . . ?
N1 Ir1 C3 C2 -13.4(7) . . . . ?
Cl1 Ir1 C3 C2 -104.6(5) . . . . ?
Cl2 Ir1 C3 C2 165.8(4) . . . . ?
C2 Ir1 C3 C8 120.2(10) . . . . ?
C1 Ir1 C3 C8 158.4(9) . . . . ?
C5 Ir1 C3 C8 -158.2(9) . . . . ?
C4 Ir1 C3 C8 -120.7(10) . . . . ?
N1 Ir1 C3 C8 106.9(9) . . . . ?
Cl1 Ir1 C3 C8 15.7(8) . . . . ?
Cl2 Ir1 C3 C8 -74.0(9) . . . . ?
C2 C3 C4 C5 0.6(9) . . . . ?
C8 C3 C4 C5 -177.6(8) . . . . ?
Ir1 C3 C4 C5 60.1(6) . . . . ?
C2 C3 C4 C9 177.3(8) . . . . ?
C8 C3 C4 C9 -1.0(14) . . . . ?
Ir1 C3 C4 C9 -123.3(8) . . . . ?
C2 C3 C4 Ir1 -59.5(5) . . . . ?
C8 C3 C4 Ir1 122.3(9) . . . . ?
C2 Ir1 C4 C3 37.8(5) . . . . ?
C1 Ir1 C4 C3 80.7(5) . . . . ?
C5 Ir1 C4 C3 119.2(7) . . . . ?
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N1 Ir1 C4 C3 113.6(7) . . . . ?
Cl1 Ir1 C4 C3 -52.9(5) . . . . ?
Cl2 Ir1 C4 C3 -142.5(5) . . . . ?
C2 Ir1 C4 C5 -81.3(5) . . . . ?
C1 Ir1 C4 C5 -38.5(5) . . . . ?
C3 Ir1 C4 C5 -119.2(7) . . . . ?
N1 Ir1 C4 C5 -5.6(9) . . . . ?
Cl1 Ir1 C4 C5 -172.1(4) . . . . ?
Cl2 Ir1 C4 C5 98.4(5) . . . . ?
C2 Ir1 C4 C9 158.4(9) . . . . ?
C1 Ir1 C4 C9 -158.8(9) . . . . ?
C5 Ir1 C4 C9 -120.3(10) . . . . ?
C3 Ir1 C4 C9 120.6(10) . . . . ?
N1 Ir1 C4 C9 -125.8(8) . . . . ?
Cl1 Ir1 C4 C9 67.6(8) . . . . ?
Cl2 Ir1 C4 C9 -21.9(8) . . . . ?
C2 C1 C5 C4 -1.9(9) . . . . ?
C6 C1 C5 C4 177.5(7) . . . . ?
Ir1 C1 C5 C4 -61.6(5) . . . . ?
C2 C1 C5 C10 -176.5(8) . . . . ?
C6 C1 C5 C10 2.9(13) . . . . ?
Ir1 C1 C5 C10 123.8(9) . . . . ?
C2 C1 C5 Ir1 59.7(5) . . . . ?
C6 C1 C5 Ir1 -120.9(8) . . . . ?
C3 C4 C5 C1 0.8(9) . . . . ?
C9 C4 C5 C1 -175.8(8) . . . . ?
Ir1 C4 C5 C1 61.4(5) . . . . ?
C3 C4 C5 C10 175.4(8) . . . . ?
C9 C4 C5 C10 -1.3(14) . . . . ?
Ir1 C4 C5 C10 -124.0(9) . . . . ?
C3 C4 C5 Ir1 -60.6(6) . . . . ?
C9 C4 C5 Ir1 122.8(9) . . . . ?
C2 Ir1 C5 C1 -36.3(5) . . . . ?
C4 Ir1 C5 C1 -116.6(7) . . . . ?
C3 Ir1 C5 C1 -80.1(5) . . . . ?
N1 Ir1 C5 C1 60.5(5) . . . . ?
Cl1 Ir1 C5 C1 -97.4(7) . . . . ?
Cl2 Ir1 C5 C1 157.0(4) . . . . ?
C2 Ir1 C5 C4 80.3(5) . . . . ?
C1 Ir1 C5 C4 116.6(7) . . . . ?
C3 Ir1 C5 C4 36.5(5) . . . . ?
N1 Ir1 C5 C4 177.2(4) . . . . ?
Cl1 Ir1 C5 C4 19.3(9) . . . . ?
Cl2 Ir1 C5 C4 -86.4(5) . . . . ?
C2 Ir1 C5 C10 -157.9(9) . . . . ?
C1 Ir1 C5 C10 -121.5(10) . . . . ?
C4 Ir1 C5 C10 121.8(10) . . . . ?
C3 Ir1 C5 C10 158.4(9) . . . . ?
N1 Ir1 C5 C10 -61.0(9) . . . . ?
Cl1 Ir1 C5 C10 141.1(7) . . . . ?
Cl2 Ir1 C5 C10 35.5(8) . . . . ?
C15 N1 C11 N2 -177.7(8) . . . . ?
Ir1 N1 C11 N2 22.1(10) . . . . ?
C15 N1 C11 C12 4.5(12) . . . . ?
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Ir1 N1 C11 C12 -155.7(6) . . . . ?
N2 C11 C12 C13 -179.8(9) . . . . ?
N1 C11 C12 C13 -2.2(13) . . . . ?
N2 C11 C12 N3 -1.4(14) . . . . ?
N1 C11 C12 N3 176.3(8) . . . . ?
O1 N3 C12 C13 174.8(11) . . . . ?
O2 N3 C12 C13 -2.4(15) . . . . ?
O1 N3 C12 C11 -3.8(16) . . . . ?
O2 N3 C12 C11 179.1(11) . . . . ?
C11 C12 C13 C14 -0.9(14) . . . . ?
N3 C12 C13 C14 -179.5(9) . . . . ?
C12 C13 C14 C15 1.6(14) . . . . ?
C11 N1 C15 C14 -4.1(13) . . . . ?
Ir1 N1 C15 C14 157.6(7) . . . . ?
C13 C14 C15 N1 0.9(14) . . . . ?

_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              26.37
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    1.496
_refine_diff_density_min   -2.877
_refine_diff_density_rms    0.154
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