```
data_pbca

_audit_creation_method            SHELXL-97
_chemical_name_systematic
;
 ?
;
_chemical_name_common             ?
_chemical_melting_point           ?
_chemical_formula_moiety          ?
_chemical_formula_sum
 'C15 H20 Cl2 N3 O2 Rh'
_chemical_formula_weight          448.15

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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'
 'Rh'  'Rh'  -1.1178   0.9187
 '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
 'x, y, z'
 '-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                    7.3892(15)
_cell_length_b                    15.071(3)
_cell_length_c                    31.125(6)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
```

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_cell_angle_gamma                 90.00
_cell_volume                      3466.2(12)
_cell_formula_units_Z             8
_cell_measurement_temperature     293(2)
_cell_measurement_reflns_used     83581
_cell_measurement_theta_min       1.30
_cell_measurement_theta_max       24.90

_exptl_crystal_description        Block
_exptl_crystal_colour             Orange
_exptl_crystal_size_max           0.3387
_exptl_crystal_size_mid           0.3259
_exptl_crystal_size_min           0.2720
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.718
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              1808
_exptl_absorpt_coefficient_mu     1.305
_exptl_absorpt_correction_type    Numerical
_exptl_absorpt_correction_T_min   0.6766
_exptl_absorpt_correction_T_max   0.7548
_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             76975
_diffrn_reflns_av_R_equivalents   0.0276
_diffrn_reflns_av_sigmaI/netI     0.0113
_diffrn_reflns_limit_h_min        -8
_diffrn_reflns_limit_h_max        8
_diffrn_reflns_limit_k_min        -17
_diffrn_reflns_limit_k_max        17
_diffrn_reflns_limit_l_min        -36
_diffrn_reflns_limit_l_max        36
_diffrn_reflns_theta_min          1.31
_diffrn_reflns_theta_max          24.87
_reflns_number_total              2993
_reflns_number_gt                 2582
_reflns_threshold_expression      >2sigma(I)
```

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_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)'
_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^)+(0.0253P)^2^+1.5417P] 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        ?
_refine_ls_number_reflns          2993
_refine_ls_number_parameters      213
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0295
_refine_ls_R_factor_gt            0.0206
_refine_ls_wR_factor_ref          0.0485
_refine_ls_wR_factor_gt           0.0464
_refine_ls_goodness_of_fit_ref    1.044
_refine_ls_restrained_S_all       1.044
_refine_ls_shift/su_max           0.002
_refine_ls_shift/su_mean          0.000

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 _atom_site_U_iso_or_equiv
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Rh1 Rh 0.14898(2) 0.787562(11) 0.399225(5) 0.03036(7) Uani 1 1 d . . .
Cl1 Cl 0.38018(9) 0.67896(4) 0.38591(2) 0.04560(16) Uani 1 1 d . . .
Cl2 Cl 0.37810(9) 0.88957(4) 0.42513(2) 0.04699(16) Uani 1 1 d . . .
O1 O 0.0466(5) 1.08085(15) 0.28560(8) 0.1019(10) Uani 1 1 d . . .
O2 O 0.0129(5) 1.02871(17) 0.22315(8) 0.1184(12) Uani 1 1 d . . .
N1 N 0.1750(3) 0.83057(12) 0.33182(6) 0.0357(4) Uani 1 1 d . . .
N2 N 0.1612(3) 0.97813(13) 0.34892(7) 0.0518(6) Uani 1 1 d . . .
H2A H 0.1911 0.9639 0.3747 0.062 Uiso 1 1 calc R . .
H2B H 0.1427 1.0328 0.3424 0.062 Uiso 1 1 calc R . .
N3 N 0.0497(4) 1.01943(17) 0.26077(8) 0.0655(7) Uani 1 1 d . . .
C1 C -0.1417(3) 0.79789(16) 0.39409(7) 0.0379(5) Uani 1 1 d . . .
C2 C -0.0883(3) 0.70682(15) 0.39979(8) 0.0385(5) Uani 1 1 d . . .
C3 C -0.0011(3) 0.69979(15) 0.44067(8) 0.0378(5) Uani 1 1 d . . .
C4 C 0.0066(3) 0.78595(15) 0.45945(7) 0.0363(5) Uani 1 1 d . . .
C5 C -0.0796(3) 0.84709(14) 0.43035(7) 0.0343(5) Uani 1 1 d . . .
C6 C -0.2451(4) 0.8330(2) 0.35706(8) 0.0531(7) Uani 1 1 d . . .
H6A H -0.2098 0.8022 0.3314 0.080 Uiso 1 1 calc R . .
H6B H -0.2205 0.8952 0.3538 0.080 Uiso 1 1 calc R . .
H6C H -0.3722 0.8245 0.3620 0.080 Uiso 1 1 calc R . .
C7 C -0.1324(4) 0.63153(19) 0.37003(9) 0.0587(8) Uani 1 1 d . . .
H7A H -0.0454 0.5848 0.3738 0.088 Uiso 1 1 calc R . .
H7B H -0.1286 0.6521 0.3409 0.088 Uiso 1 1 calc R . .
H7C H -0.2513 0.6095 0.3764 0.088 Uiso 1 1 calc R . .
C8 C 0.0664(4) 0.61646(17) 0.46105(10) 0.0577(8) Uani 1 1 d . . .
H8A H 0.1713 0.6295 0.4781 0.086 Uiso 1 1 calc R . .
H8B H 0.0979 0.5745 0.4391 0.086 Uiso 1 1 calc R . .
H8C H -0.0265 0.5919 0.4790 0.086 Uiso 1 1 calc R . .
C9 C 0.0817(4) 0.80771(19) 0.50246(8) 0.0520(7) Uani 1 1 d . . .
H9A H -0.0155 0.8135 0.5227 0.078 Uiso 1 1 calc R . .
H9B H 0.1474 0.8626 0.5009 0.078 Uiso 1 1 calc R . .
H9C H 0.1616 0.7611 0.5115 0.078 Uiso 1 1 calc R . .
C10 C -0.1106(4) 0.94346(16) 0.43899(9) 0.0527(7) Uani 1 1 d . . .
H10A H -0.1230 0.9746 0.4122 0.079 Uiso 1 1 calc R . .
H10B H -0.0096 0.9671 0.4547 0.079 Uiso 1 1 calc R . .
H10C H -0.2191 0.9506 0.4556 0.079 Uiso 1 1 calc R . .
C11 C 0.1437(3) 0.91600(15) 0.31930(7) 0.0381(5) Uani 1 1 d . . .
C12 C 0.0932(4) 0.93094(16) 0.27621(8) 0.0433(6) Uani 1 1 d . . .
C13 C 0.0803(4) 0.86176(19) 0.24737(8) 0.0518(7) Uani 1 1 d . . .
H13 H 0.0449 0.8724 0.2192 0.062 Uiso 1 1 calc R . .
C14 C 0.1195(4) 0.77791(18) 0.26044(8) 0.0514(7) Uani 1 1 d . . .
H14 H 0.1147 0.7306 0.2413 0.062 Uiso 1 1 calc R . .
C15 C 0.1665(3) 0.76493(16) 0.30286(8) 0.0424(6) Uani 1 1 d . . .
H15 H 0.1937 0.7076 0.3118 0.051 Uiso 1 1 calc R . .

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 _atom_site_aniso_U_11
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 _atom_site_aniso_U_23
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Rh1 0.03416(11) 0.02496(10) 0.03197(10) -0.00206(7) 0.00315(8) -
0.00121(8)
Cl1 0.0421(4) 0.0364(3) 0.0583(4) -0.0066(3) 0.0052(3) 0.0067(3)
Cl2 0.0490(4) 0.0397(3) 0.0523(4) -0.0062(3) -0.0059(3) -0.0106(3)
O1 0.184(3) 0.0463(13) 0.0750(16) 0.0057(12) -0.0367(18) 0.0175(17)
O2 0.219(4) 0.0797(17) 0.0565(15) 0.0256(13) -0.0354(19) -0.005(2)
N1 0.0424(12) 0.0310(10) 0.0338(10) -0.0023(8) 0.0059(9) -0.0044(9)
N2 0.0871(18) 0.0284(10) 0.0398(11) 0.0008(9) -0.0045(12) -0.0011(11)
N3 0.094(2) 0.0540(15) 0.0480(15) 0.0162(12) -0.0115(14) -0.0064(15)
C1 0.0319(12) 0.0444(14) 0.0374(12) 0.0024(10) 0.0051(10) 0.0005(11)
C2 0.0367(13) 0.0366(13) 0.0423(13) -0.0055(11) 0.0092(11) -0.0088(11)
C3 0.0395(14) 0.0318(12) 0.0420(13) 0.0050(10) 0.0119(11) 0.0013(10)
C4 0.0370(13) 0.0386(13) 0.0333(12) 0.0000(10) 0.0071(10) 0.0014(11)
C5 0.0351(12) 0.0332(12) 0.0345(12) 0.0003(9) 0.0055(10) 0.0043(10)
C6 0.0426(15) 0.0735(19) 0.0432(14) 0.0074(13) -0.0039(13) 0.0008(14)
C7 0.0571(18) 0.0518(16) 0.0671(19) -0.0216(14) 0.0102(15) -0.0187(15)
C8 0.0667(19) 0.0388(14) 0.0675(18) 0.0176(13) 0.0176(16) 0.0072(14)
C9 0.0561(17) 0.0652(18) 0.0348(13) -0.0030(12) -0.0009(13) 0.0056(14)
C10 0.0628(19) 0.0373(14) 0.0579(16) -0.0017(12) 0.0126(14) 0.0116(13)
C11 0.0428(14) 0.0334(12) 0.0379(12) 0.0025(10) 0.0064(11) -0.0050(11)
C12 0.0501(16) 0.0426(13) 0.0371(13) 0.0049(11) 0.0026(11) -0.0062(12)
C13 0.0563(17) 0.0654(17) 0.0338(13) 0.0007(13) 0.0036(12) -0.0093(15)
C14 0.0607(19) 0.0524(16) 0.0410(14) -0.0135(12) 0.0077(12) -0.0087(14)
C15 0.0489(15) 0.0361(13) 0.0423(14) -0.0052(10) 0.0105(12) -0.0050(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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 _geom_bond_atom_site_label_2
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Rh1 C2 2.134(2) . ?
Rh1 C5 2.144(2) . ?
Rh1 C4 2.150(2) . ?
Rh1 C3 2.155(2) . ?
Rh1 C1 2.159(2) . ?
```

```
Rh1 N1 2.2043(19) . ?
Rh1 Cl1 2.4020(7) . ?
Rh1 Cl2 2.4249(7) . ?
O1 N3 1.206(3) . ?
O2 N3 1.210(3) . ?
N1 C15 1.340(3) . ?
N1 C11 1.365(3) . ?
N2 C11 1.320(3) . ?
N2 H2A 0.8600 . ?
N2 H2B 0.8600 . ?
N3 C12 1.454(3) . ?
C1 C5 1.426(3) . ?
C1 C2 1.439(3) . ?
C1 C6 1.481(3) . ?
C2 C3 1.430(3) . ?
C2 C7 1.501(3) . ?
C3 C4 1.425(3) . ?
C3 C8 1.493(3) . ?
C4 C5 1.440(3) . ?
C4 C9 1.486(3) . ?
C5 C10 1.495(3) . ?
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 1.410(3) . ?
C12 C13 1.379(4) . ?
C13 C14 1.359(4) . ?
C13 H13 0.9300 . ?
C14 C15 1.379(4) . ?
C14 H14 0.9300 . ?
C15 H15 0.9300 . ?

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C2 Rh1 C5 65.65(9) . . ?
C2 Rh1 C4 65.44(9) . . ?
```

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C5 Rh1 C4 39.20(8) . . ?
C2 Rh1 C3 38.95(9) . . ?
C5 Rh1 C3 65.23(8) . . ?
C4 Rh1 C3 38.67(9) . . ?
C2 Rh1 C1 39.16(9) . . ?
C5 Rh1 C1 38.71(9) . . ?
C4 Rh1 C1 65.07(9) . . ?
C3 Rh1 C1 64.96(9) . . ?
C2 Rh1 N1 104.31(8) . . ?
C5 Rh1 N1 112.08(8) . . ?
C4 Rh1 N1 151.16(8) . . ?
C3 Rh1 N1 142.68(8) . . ?
C1 Rh1 N1 89.73(8) . . ?
C2 Rh1 Cl1 101.37(7) . . ?
C5 Rh1 Cl1 157.44(6) . . ?
C4 Rh1 Cl1 119.40(6) . . ?
C3 Rh1 Cl1 92.92(6) . . ?
C1 Rh1 Cl1 138.06(7) . . ?
N1 Rh1 Cl1 88.51(5) . . ?
C2 Rh1 Cl2 158.80(6) . . ?
C5 Rh1 Cl2 97.73(7) . . ?
C4 Rh1 Cl2 93.38(7) . . ?
C3 Rh1 Cl2 123.33(7) . . ?
C1 Rh1 Cl2 132.33(7) . . ?
N1 Rh1 Cl2 93.96(5) . . ?
Cl1 Rh1 Cl2 89.59(3) . . ?
C15 N1 C11 119.8(2) . . ?
C15 N1 Rh1 114.77(15) . . ?
C11 N1 Rh1 122.29(14) . . ?
C11 N2 H2A 120.0 . . ?
C11 N2 H2B 120.0 . . ?
H2A N2 H2B 120.0 . . ?
O1 N3 O2 121.8(3) . . ?
O1 N3 C12 119.8(2) . . ?
O2 N3 C12 118.4(3) . . ?
C5 C1 C2 108.1(2) . . ?
C5 C1 C6 126.6(2) . . ?
C2 C1 C6 125.4(2) . . ?
C5 C1 Rh1 70.07(13) . . ?
C2 C1 Rh1 69.48(14) . . ?
C6 C1 Rh1 126.65(17) . . ?
C3 C2 C1 107.69(19) . . ?
C3 C2 C7 126.2(2) . . ?
C1 C2 C7 125.9(2) . . ?
C3 C2 Rh1 71.30(13) . . ?
C1 C2 Rh1 71.35(13) . . ?
C7 C2 Rh1 127.18(18) . . ?
C4 C3 C2 108.4(2) . . ?
C4 C3 C8 125.4(2) . . ?
C2 C3 C8 126.2(2) . . ?
C4 C3 Rh1 70.48(13) . . ?
C2 C3 Rh1 69.75(13) . . ?
C8 C3 Rh1 126.80(18) . . ?
C3 C4 C5 107.9(2) . . ?
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C3 C4 C9 125.8(2) . . ?
C5 C4 C9 126.2(2) . . ?
C3 C4 Rh1 70.85(13) . . ?
C5 C4 Rh1 70.18(12) . . ?
C9 C4 Rh1 126.90(18) . . ?
C1 C5 C4 107.9(2) . . ?
C1 C5 C10 126.7(2) . . ?
C4 C5 C10 125.2(2) . . ?
C1 C5 Rh1 71.22(13) . . ?
C4 C5 Rh1 70.61(13) . . ?
C10 C5 Rh1 127.48(18) . . ?
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 116.9(2) . . ?
N2 C11 C12 125.2(2) . . ?
N1 C11 C12 117.8(2) . . ?
C13 C12 C11 121.1(2) . . ?
C13 C12 N3 117.6(2) . . ?
C11 C12 N3 121.3(2) . . ?
C14 C13 C12 119.6(2) . . ?
C14 C13 H13 120.2 . . ?
C12 C13 H13 120.2 . . ?
C13 C14 C15 118.2(2) . . ?
C13 C14 H14 120.9 . . ?
C15 C14 H14 120.9 . . ?
N1 C15 C14 123.4(2) . . ?
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N1 C15 H15 118.3 . . ?
C14 C15 H15 118.3 . . ?

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C5 Rh1 N1 C15 -119.82(18) . . . . ?
C4 Rh1 N1 C15 -115.4(2) . . . . ?
C3 Rh1 N1 C15 -42.2(2) . . . . ?
C1 Rh1 N1 C15 -87.39(18) . . . . ?
Cl1 Rh1 N1 C15 50.70(17) . . . . ?
Cl2 Rh1 N1 C15 140.18(17) . . . . ?
C2 Rh1 N1 C11 109.13(19) . . . . ?
C5 Rh1 N1 C11 40.0(2) . . . . ?
C4 Rh1 N1 C11 44.3(3) . . . . ?
C3 Rh1 N1 C11 117.6(2) . . . . ?
C1 Rh1 N1 C11 72.40(19) . . . . ?
Cl1 Rh1 N1 C11 -149.51(18) . . . . ?
Cl2 Rh1 N1 C11 -60.02(19) . . . . ?
C2 Rh1 C1 C5 119.21(19) . . . . ?
C4 Rh1 C1 C5 38.14(13) . . . . ?
C3 Rh1 C1 C5 80.99(14) . . . . ?
N1 Rh1 C1 C5 -127.38(13) . . . . ?
Cl1 Rh1 C1 C5 145.16(11) . . . . ?
Cl2 Rh1 C1 C5 -32.27(16) . . . . ?
C5 Rh1 C1 C2 -119.21(19) . . . . ?
C4 Rh1 C1 C2 -81.07(14) . . . . ?
C3 Rh1 C1 C2 -38.22(13) . . . . ?
N1 Rh1 C1 C2 113.42(13) . . . . ?
Cl1 Rh1 C1 C2 25.95(17) . . . . ?
Cl2 Rh1 C1 C2 -151.47(11) . . . . ?
C2 Rh1 C1 C6 -119.4(3) . . . . ?
C5 Rh1 C1 C6 121.3(3) . . . . ?
C4 Rh1 C1 C6 159.5(3) . . . . ?
C3 Rh1 C1 C6 -157.7(3) . . . . ?
N1 Rh1 C1 C6 -6.0(2) . . . . ?
Cl1 Rh1 C1 C6 -93.5(2) . . . . ?
Cl2 Rh1 C1 C6 89.1(2) . . . . ?
C5 C1 C2 C3 2.8(3) . . . . ?
C6 C1 C2 C3 -176.5(2) . . . . ?
Rh1 C1 C2 C3 62.43(16) . . . . ?
C5 C1 C2 C7 177.4(2) . . . . ?
C6 C1 C2 C7 -1.8(4) . . . . ?
Rh1 C1 C2 C7 -122.9(2) . . . . ?
C5 C1 C2 Rh1 -59.67(16) . . . . ?
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C6 C1 C2 Rh1 121.1(2) . . . . ?
C5 Rh1 C2 C3 -80.11(14) . . . . ?
C4 Rh1 C2 C3 -36.86(13) . . . . ?
C1 Rh1 C2 C3 -116.92(19) . . . . ?
N1 Rh1 C2 C3 171.81(12) . . . . ?
Cl1 Rh1 C2 C3 80.43(13) . . . . ?
Cl2 Rh1 C2 C3 -39.4(3) . . . . ?
C5 Rh1 C2 C1 36.81(13) . . . . ?
C4 Rh1 C2 C1 80.06(14) . . . . ?
C3 Rh1 C2 C1 116.92(19) . . . . ?
N1 Rh1 C2 C1 -71.27(14) . . . . ?
Cl1 Rh1 C2 C1 -162.64(12) . . . . ?
Cl2 Rh1 C2 C1 77.5(2) . . . . ?
C5 Rh1 C2 C7 158.1(3) . . . . ?
C4 Rh1 C2 C7 -158.6(3) . . . . ?
C3 Rh1 C2 C7 -121.8(3) . . . . ?
C1 Rh1 C2 C7 121.3(3) . . . . ?
N1 Rh1 C2 C7 50.1(3) . . . . ?
Cl1 Rh1 C2 C7 -41.3(2) . . . . ?
Cl2 Rh1 C2 C7 -161.20(17) . . . . ?
C1 C2 C3 C4 -2.3(3) . . . . ?
C7 C2 C3 C4 -177.0(2) . . . . ?
Rh1 C2 C3 C4 60.14(16) . . . . ?
C1 C2 C3 C8 176.1(2) . . . . ?
C7 C2 C3 C8 1.5(4) . . . . ?
Rh1 C2 C3 C8 -121.4(3) . . . . ?
C1 C2 C3 Rh1 -62.47(16) . . . . ?
C7 C2 C3 Rh1 122.9(3) . . . . ?
C2 Rh1 C3 C4 -119.2(2) . . . . ?
C5 Rh1 C3 C4 -37.88(14) . . . . ?
C1 Rh1 C3 C4 -80.75(15) . . . . ?
N1 Rh1 C3 C4 -132.33(15) . . . . ?
Cl1 Rh1 C3 C4 136.30(13) . . . . ?
Cl2 Rh1 C3 C4 44.87(16) . . . . ?
C5 Rh1 C3 C2 81.28(15) . . . . ?
C4 Rh1 C3 C2 119.2(2) . . . . ?
C1 Rh1 C3 C2 38.42(13) . . . . ?
N1 Rh1 C3 C2 -13.2(2) . . . . ?
Cl1 Rh1 C3 C2 -104.54(13) . . . . ?
Cl2 Rh1 C3 C2 164.04(11) . . . . ?
C2 Rh1 C3 C8 120.7(3) . . . . ?
C5 Rh1 C3 C8 -158.0(3) . . . . ?
C4 Rh1 C3 C8 -120.1(3) . . . . ?
C1 Rh1 C3 C8 159.1(3) . . . . ?
N1 Rh1 C3 C8 107.5(2) . . . . ?
Cl1 Rh1 C3 C8 16.2(2) . . . . ?
Cl2 Rh1 C3 C8 -75.3(2) . . . . ?
C2 C3 C4 C5 1.0(3) . . . . ?
C8 C3 C4 C5 -177.4(2) . . . . ?
Rh1 C3 C4 C5 60.71(16) . . . . ?
C2 C3 C4 C9 178.1(2) . . . . ?
C8 C3 C4 C9 -0.4(4) . . . . ?
Rh1 C3 C4 C9 -122.2(2) . . . . ?
C2 C3 C4 Rh1 -59.68(16) . . . . ?
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C8 C3 C4 Rh1 121.9(3) . . . . ?
C2 Rh1 C4 C3 37.13(14) . . . . ?
C5 Rh1 C4 C3 118.1(2) . . . . ?
C1 Rh1 C4 C3 80.44(15) . . . . ?
N1 Rh1 C4 C3 111.68(18) . . . . ?
Cl1 Rh1 C4 C3 -52.38(15) . . . . ?
Cl2 Rh1 C4 C3 -143.81(13) . . . . ?
C2 Rh1 C4 C5 -80.97(15) . . . . ?
C3 Rh1 C4 C5 -118.1(2) . . . . ?
C1 Rh1 C4 C5 -37.66(13) . . . . ?
N1 Rh1 C4 C5 -6.4(2) . . . . ?
Cl1 Rh1 C4 C5 -170.47(11) . . . . ?
Cl2 Rh1 C4 C5 98.09(13) . . . . ?
C2 Rh1 C4 C9 158.1(2) . . . . ?
C5 Rh1 C4 C9 -120.9(3) . . . . ?
C3 Rh1 C4 C9 121.0(3) . . . . ?
C1 Rh1 C4 C9 -158.6(2) . . . . ?
N1 Rh1 C4 C9 -127.4(2) . . . . ?
Cl1 Rh1 C4 C9 68.6(2) . . . . ?
Cl2 Rh1 C4 C9 -22.9(2) . . . . ?
C2 C1 C5 C4 -2.1(3) . . . . ?
C6 C1 C5 C4 177.1(2) . . . . ?
Rh1 C1 C5 C4 -61.43(16) . . . . ?
C2 C1 C5 C10 -177.4(2) . . . . ?
C6 C1 C5 C10 1.8(4) . . . . ?
Rh1 C1 C5 C10 123.2(2) . . . . ?
C2 C1 C5 Rh1 59.31(16) . . . . ?
C6 C1 C5 Rh1 -121.4(2) . . . . ?
C3 C4 C5 C1 0.7(3) . . . . ?
C9 C4 C5 C1 -176.4(2) . . . . ?
Rh1 C4 C5 C1 61.82(16) . . . . ?
C3 C4 C5 C10 176.1(2) . . . . ?
C9 C4 C5 C10 -1.0(4) . . . . ?
Rh1 C4 C5 C10 -122.8(2) . . . . ?
C3 C4 C5 Rh1 -61.13(16) . . . . ?
C9 C4 C5 Rh1 121.8(2) . . . . ?
C2 Rh1 C5 C1 -37.23(13) . . . . ?
C4 Rh1 C5 C1 -117.62(19) . . . . ?
C3 Rh1 C5 C1 -80.24(15) . . . . ?
N1 Rh1 C5 C1 59.04(14) . . . . ?
Cl1 Rh1 C5 C1 -95.55(19) . . . . ?
Cl2 Rh1 C5 C1 156.53(12) . . . . ?
C2 Rh1 C5 C4 80.39(15) . . . . ?
C3 Rh1 C5 C4 37.38(14) . . . . ?
C1 Rh1 C5 C4 117.62(19) . . . . ?
N1 Rh1 C5 C4 176.66(12) . . . . ?
Cl1 Rh1 C5 C4 22.1(2) . . . . ?
Cl2 Rh1 C5 C4 -85.85(13) . . . . ?
C2 Rh1 C5 C10 -159.6(2) . . . . ?
C4 Rh1 C5 C10 120.0(3) . . . . ?
C3 Rh1 C5 C10 157.4(2) . . . . ?
C1 Rh1 C5 C10 -122.4(3) . . . . ?
N1 Rh1 C5 C10 -63.3(2) . . . . ?
Cl1 Rh1 C5 C10 142.07(18) . . . . ?
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Cl2 Rh1 C5 C10 34.1(2) . . . . ?
C15 N1 C11 N2 -177.3(2) . . . . ?
Rh1 N1 C11 N2 23.8(3) . . . . ?
C15 N1 C11 C12 3.4(3) . . . . ?
Rh1 N1 C11 C12 -155.41(18) . . . . ?
N2 C11 C12 C13 179.3(3) . . . . ?
N1 C11 C12 C13 -1.5(4) . . . . ?
N2 C11 C12 N3 -1.9(4) . . . . ?
N1 C11 C12 N3 177.3(2) . . . . ?
O1 N3 C12 C13 174.7(3) . . . . ?
O2 N3 C12 C13 -3.5(5) . . . . ?
O1 N3 C12 C11 -4.1(5) . . . . ?
O2 N3 C12 C11 177.7(3) . . . . ?
C11 C12 C13 C14 -1.1(4) . . . . ?
N3 C12 C13 C14 -179.9(3) . . . . ?
C12 C13 C14 C15 1.7(4) . . . . ?
C11 N1 C15 C14 -2.9(4) . . . . ?
Rh1 N1 C15 C14 157.5(2) . . . . ?
C13 C14 C15 N1 0.2(4) . . . . ?

_diffrn_measured_fraction_theta_max    0.996
_diffrn_reflns_theta_full              24.87
_diffrn_measured_fraction_theta_full   0.996
_refine_diff_density_max    0.342
_refine_diff_density_min   -0.280
_refine_diff_density_rms    0.045
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