checkCIF/PLATON (full publication check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: Ket2

```
Bond precision:        C-C = 0.0048 A                  Wavelength=0.71073
Cell:         a=10.9701(11)     b=11.0589(13)     c=15.1717(15)
              alpha=74.472(9)   beta=73.584(9)    gamma=70.246(10)
Temperature: 180 K
                     Calculated                          Reported
Volume               1631.2(3)                           1631.2(3)
Space group          P -1                                P -1
Hall group           -P 1                                -P 1
Moiety formula       2(C32 H38 Cl2 N2 O2 Ru), C H4 O     2(C32 H38 Cl2 N2 O2 Ru), C H4 O
Sum formula          C65 H80 Cl4 N4 O5 Ru2               C65 H80 Cl4 N4 O5 Ru2
Mr                   1341.27                             1341.27
Dx,g cm-3            1.365                               1.365
Z                    1                                   1
Mu (mm-1)            0.676                               0.676
F000                 694.0                               694.0
F000'                692.28
h,k,lmax             13,13,18                            13,13,18
Nref                 6670                                6608
Tmin,Tmax            0.857,0.941                         0.756,0.945
Tmin'                0.784
Correction method= GAUSSIAN
Data completeness= 0.991          Theta(max)= 26.370
R(reflections)= 0.0407( 5117)         wR2(reflections)= 0.0903( 6608)
S = 1.026               Npar= 377
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

Crystal system given = triclinic
PLAT415_ALERT_2_B Short Inter D-H..H-X H5B .. H100 .. 2.09 Ang.

Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.04 Ratio

Alert level G

PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..... 100 Perc.

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
1 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: Kme2

```
Bond precision:        C-C = 0.0039 A                  Wavelength=0.71073
Cell:         a=11.913(9)       b=11.970(7)       c=15.284(10)
              alpha=106.60(4)   beta=93.07(5)     gamma=117.141(11)
Temperature: 180 K
                     Calculated                          Reported
Volume               1815(2)                             1815(2)
Space group          P -1                                P -1
Hall group           -P 1                                -P 1
Moiety formula       C31 H36 Cl2 N2 O2 Ru, 2(C H2 Cl2)   C31 H36 Cl2 N2 O2 Ru, 2(C H2 Cl2)
Sum formula          C33 H40 Cl6 N2 O2 Ru                C33 H40 Cl6 N2 O2 Ru
Mr                   810.44                              810.44
Dx,g cm-3            1.483                               1.483
Z                    2                                   2
Mu (mm-1)            0.905                               0.905
F000                 828.0                               828.0
```

F000'	827.47	
h,k,lmax	16,16,21	16,16,21
Nref	10445	10379
Tmin,Tmax	0.805,0.897	0.708,0.902
Tmin'	0.684	

Correction method= MULTI-SCAN
Data completeness= 0.994 Theta(max)= 29.830
R(reflections)= 0.0363(9554) wR2(reflections)= 0.0920(10379)
S = 1.073 Npar= 404

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C100
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1
C31 H36 Cl2 N2 O2 Ru

Alert level G

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- Cl1 .. 7.67 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- O2 .. 12.25 su
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2
C H2 Cl2

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock: M2

Bond precision: C-C = 0.0023 A Wavelength=0.71073
Cell: a=34.4881(11) b=15.1596(5) c=18.2349(6)
alpha=90 beta=116.131(1) gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	8559.2(5)	8559.2(5)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C33 H37 Cl2 N2 O5 Ru, C H2 Cl2	C33 H37 Cl2 N2 O5 Ru, 1.5(Ch2Cl2), C6H14
Sum formula	C34 H39 Cl4 N2 O5 Ru	C40.50 H54 Cl5 N2 O5 Ru
Mr	798.54	927.18
Dx,g cm-3	1.239	1.439
Z	8	8
Mu (mm-1)	0.651	0.723
F000	3272.0	3840.0
F000'	3267.75	
h,k,lmax	59,26,31	57,25,30
Nref	22938	21013
Tmin,Tmax	0.841,0.865	0.716,0.870
Tmin'	0.776	

Correction method= MULTI-SCAN
Data completeness= 0.916 Theta(max)= 37.760
R(reflections)= 0.0377(15780) wR2(reflections)= 0.1179(21013)
S = 1.116 Npar= 423

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_weight 927.18
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	34.00	408.37
H	1.01	39.00	39.31
N	14.01	2.00	28.01
O	16.00	5.00	79.99
Cl	35.45	4.00	141.81
Ru	101.07	1.00	101.07

Calculated formula weight 798.58

Author Response: After completing the initial structure solution, it was found that 21% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 0.5 molecule of CH2Cl2 and 1.0 molecule of hexane were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.92

Author Response: The data set shows a completennes of 99% for S < 0.8 A-1

PLAT043_ALERT_1_A Check Reported Molecular Weight 927.18

Author Response: After completing the initial structure solution, it was found that 21% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 0.5 molecule of CH2Cl2 and 1.0 molecule of hexane were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

PLAT044_ALERT_1_A Calculated and Reported Dx Differ ..... ?

Author Response: After completing the initial structure solution, it was found that 21% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 0.5 molecule of CH2Cl2 and 1.0 molecule of hexane were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure !

Author Response: After completing the initial structure solution, it was found that 21% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 0.5 molecule of CH2Cl2 and 1.0 molecule of hexane were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

Alert level B

PLAT051_ALERT_1_B Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 9.91 Perc.
PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.02 Ratio

Alert level C

REFLT03_ALERT_3_C Reflection count < 95% complete
From the CIF: _diffrn_reflns_theta_max 37.76
From the CIF: _diffrn_reflns_theta_full 37.76
From the CIF: _reflns_number_total 21013
TEST2: Reflns within _diffrn_reflns_theta_max
Count of symmetry unique reflns 22938
Completeness (_total/calc) 91.61%
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 4.11 Ratio
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C100

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C40.5 H54 Cl5 N2 O5 Ru1
Atom count from the _atom_site data: C34 H39 Cl4 N2 O5 Ru1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum C40.50 H54 Cl5 N2 O5 Ru
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif	sites	diff
C	324.00	272.00		52.00
H	432.00	312.00		120.00
Cl	40.00	32.00		8.00
N	16.00	16.00		0.00
O	40.00	40.00		0.00
Ru	8.00	8.00		0.00

REFLT03_ALERT_1_G ALERT: Expected hkl max differ from CIF values
From the CIF: _diffrn_reflns_theta_max 37.76
From the CIF: _reflns_number_total 21013
From the CIF: _diffrn_reflns_limit_ max hkl 52. 25. 29.
From the CIF: _diffrn_reflns_limit_ min hkl -57. -22. -30.
TEST1: Expected hkl limits for theta max
Calculated maximum hkl 59. 26. 31.
Calculated minimum hkl -59. -26. -31.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- Cl1 .. 8.94 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- Cl2 .. 10.79 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- C1 .. 6.80 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- C4 .. 10.20 su
PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C5
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl3 .. Cl3 .. 3.35 Ang.
PLAT950_ALERT_5_G Reported and Calculated Hmax Values Differ by .. 2

5 **ALERT level A** = Most likely a serious problem - resolve or explain
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6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: C2

Bond precision: C-C = 0.0029 A Wavelength=0.71073

Cell: a=11.9763(4) b=16.6003(6) c=18.6197(6)
alpha=90 beta=102.306(2) gamma=90

Temperature: 180 K

	Calculated	Reported
Volume	3616.7(2)	3616.7(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C31 H35 Cl2 N3 O Ru	C31 H33 Cl2 N2 O Ru, 2 C H2 Cl2
Sum formula	C31 H35 Cl2 N3 O Ru	C33 H37 Cl6 N2 O Ru
Mr	637.59	807.44
Dx,g cm-3	1.171	1.483
Z	4	4
Mu (mm-1)	0.604	0.907
F000	1312.0	1648.0
F000'	1308.50	
h,k,lmax	18,25,28	18,25,28
Nref	13706	13617
Tmin,Tmax	0.804,0.913	0.795,0.916
Tmin'	0.748	

Correction method= MULTI-SCAN

Data completeness= 0.994 Theta(max)= 33.050

R(reflections)= 0.0359(9924) wR2(reflections)= 0.0952(13617)

S = 1.027 Npar= 351

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 807.44
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	31.00	372.34
H	1.01	35.00	35.28
N	14.01	3.00	42.02
O	16.00	1.00	16.00
Cl	35.45	2.00	70.91
Ru	101.07	1.00	101.07

Calculated formula weight 637.62

Author Response: After completing the initial structure solution, it was found that 23% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 2 molecules of CH2Cl2 were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

PLAT043_ALERT_1_A Check Reported Molecular Weight 807.44

Author Response: After completing the initial structure solution, it was found that 23% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 2 molecules of CH2Cl2 were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

PLAT044_ALERT_1_A Calculated and Reported Dx Differ ..... ?

Author Response: After completing the initial structure solution, it was found that 23% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 2 molecules of CH2Cl2 were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 33.35 Perc.

Author Response: After completing the initial structure solution, it was found that 23% of the total cell volume was filled with disordered solvent, which could not be modelled in terms of atomic sites. The SQUEEZE procedure was applied to the data, and 2 molecules of CH2Cl2 were included in the formula, formula weight, calculated density, absorption coefficient, and F(000).

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure !

Alert level B

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 4.27 Ratio

Alert level C

CHEMW01_ALERT_1_C The ratio of given/expected molecular weight as calculated
from the _chemical_formula_sum lies outside
the range 0.99 <> 1.01
Calculated formula weight = 791.4561
Formula weight given = 807.4400
CHEMW01_ALERT_1_C The difference between the given and expected weight for
compound is greater 1 mass unit. Check that all hydrogen
atoms have been taken into account.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ ?
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ ?
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... ?
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C33 H37 Cl6 N2 O1 Ru1
Atom count from the _atom_site data: C31 H35 Cl2 N3 O1 Ru1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C33 H37 Cl6 N2 O Ru
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	132.00	124.00	8.00
H	148.00	140.00	8.00
Cl	24.00	8.00	16.00
N	8.00	12.00	-4.00
O	4.00	4.00	0.00
Ru	4.00	4.00	0.00

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- Cl1 .. 11.50 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- Cl2 .. 6.50 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- O1 .. 5.40 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- C1 .. 5.57 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ru1 -- C4 .. 5.63 su
PLAT793_ALERT_4_G The Model has Chirality at C5 (Verify) .... R

5 **ALERT level A** = Most likely a serious problem - resolve or explain
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10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
missing. This is required for a full paper submission (but is
optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
empty.

4 **ALERT level A** = Data missing that is essential or data in wrong format
2 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. *checkCIF* was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a

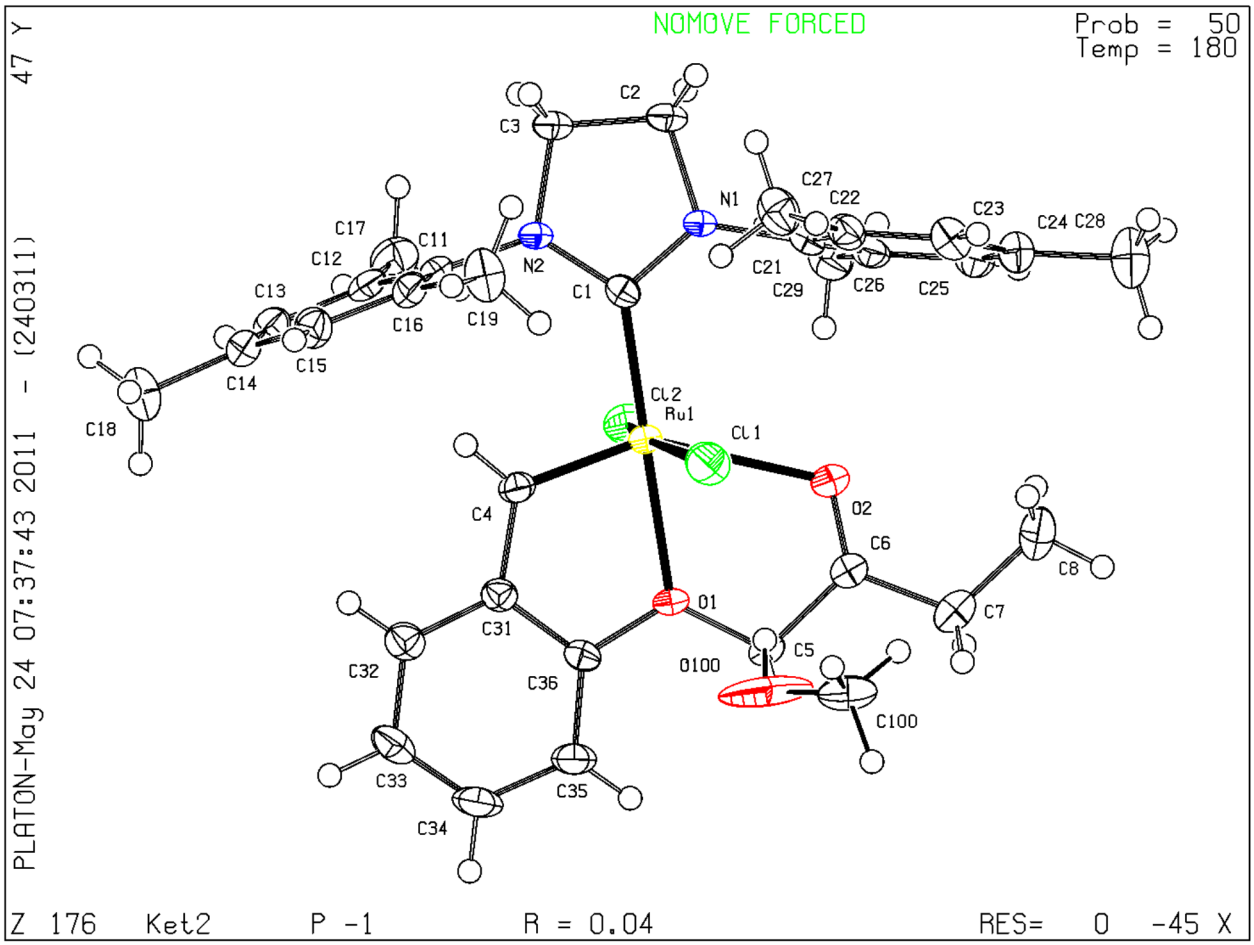
basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT602_C2
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure       !
RESPONSE: ...
;
# end Validation Reply Form
```

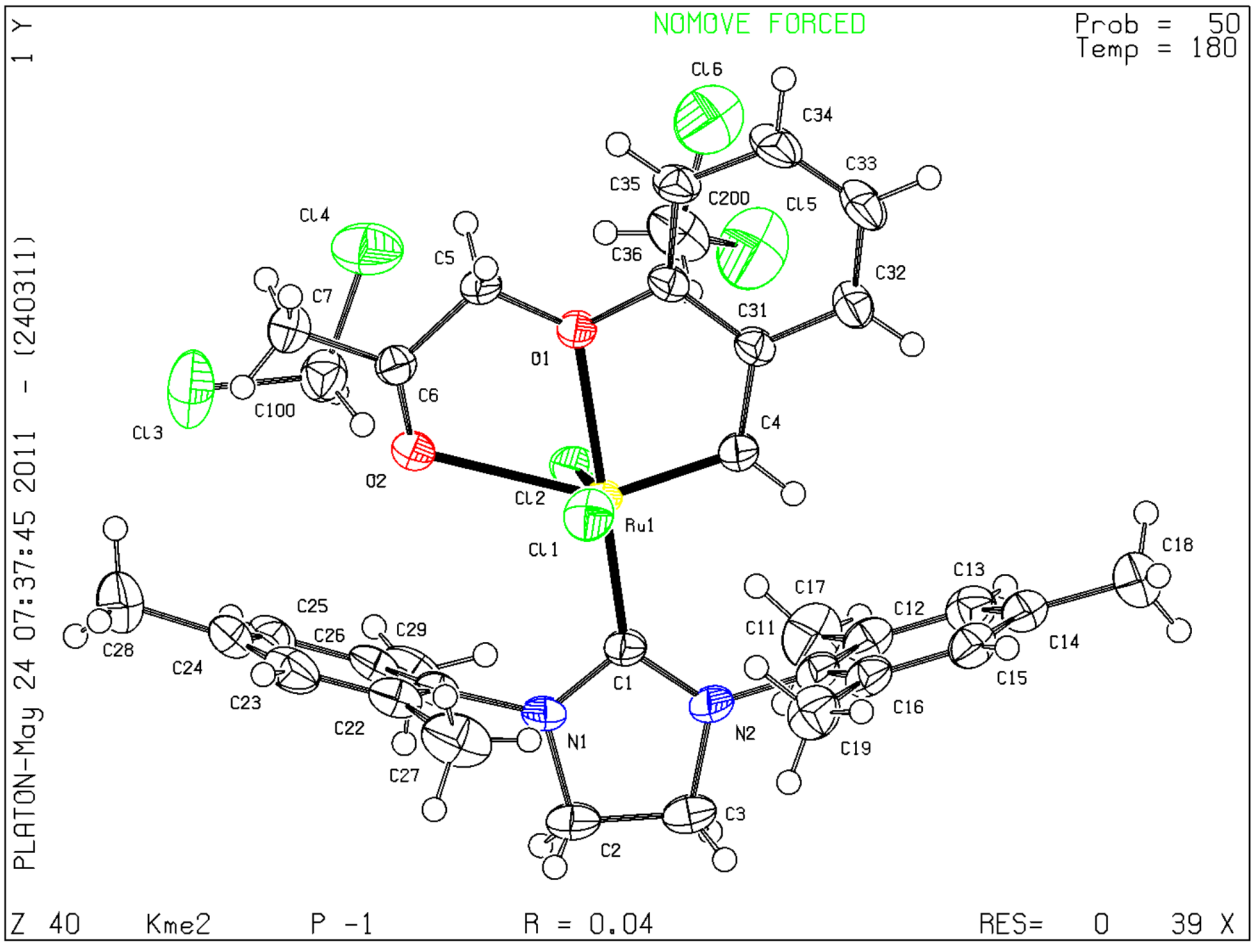
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 24/03/2011; check.def file version of 16/03/2011

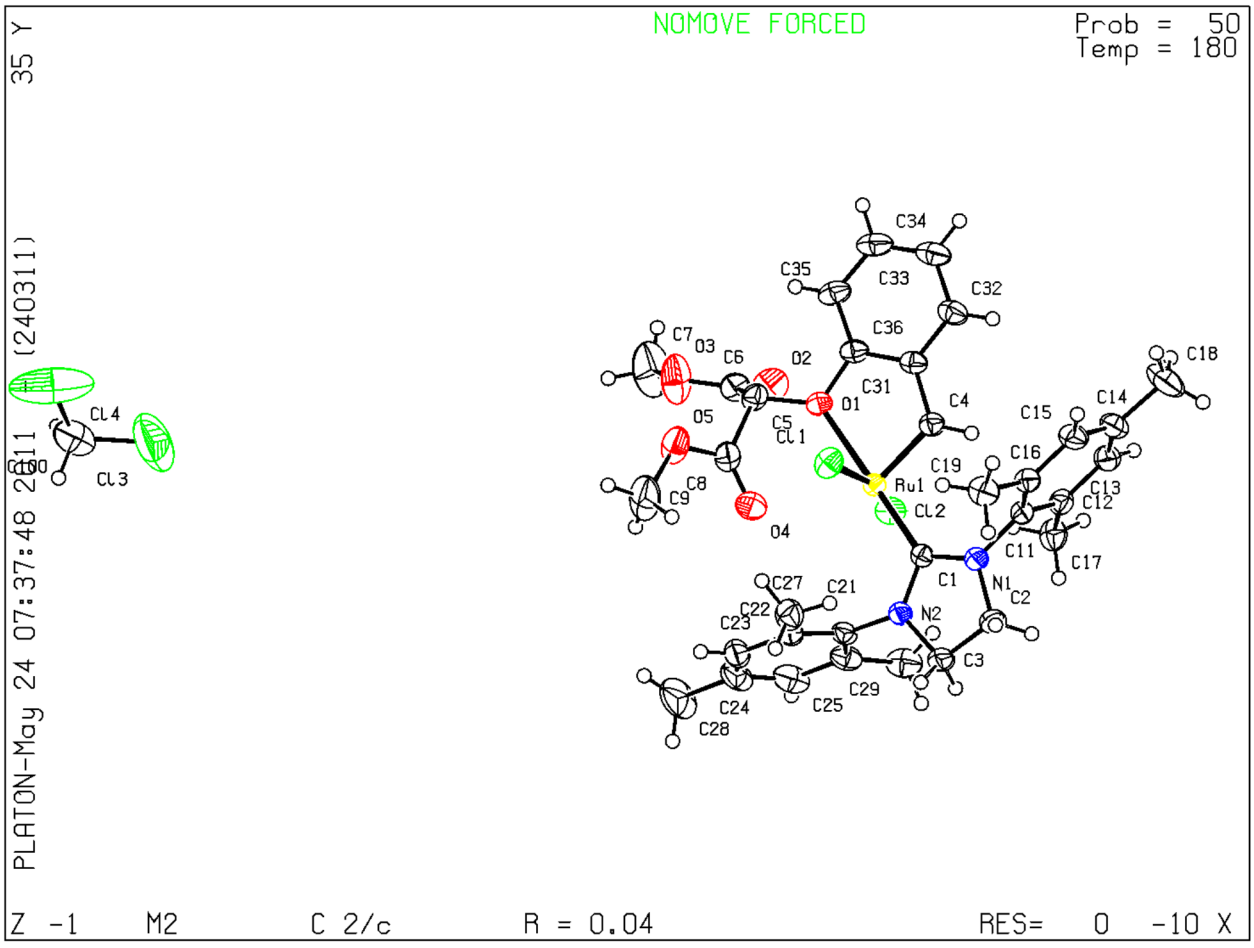
Datablock Ket2 - ellipsoid plot



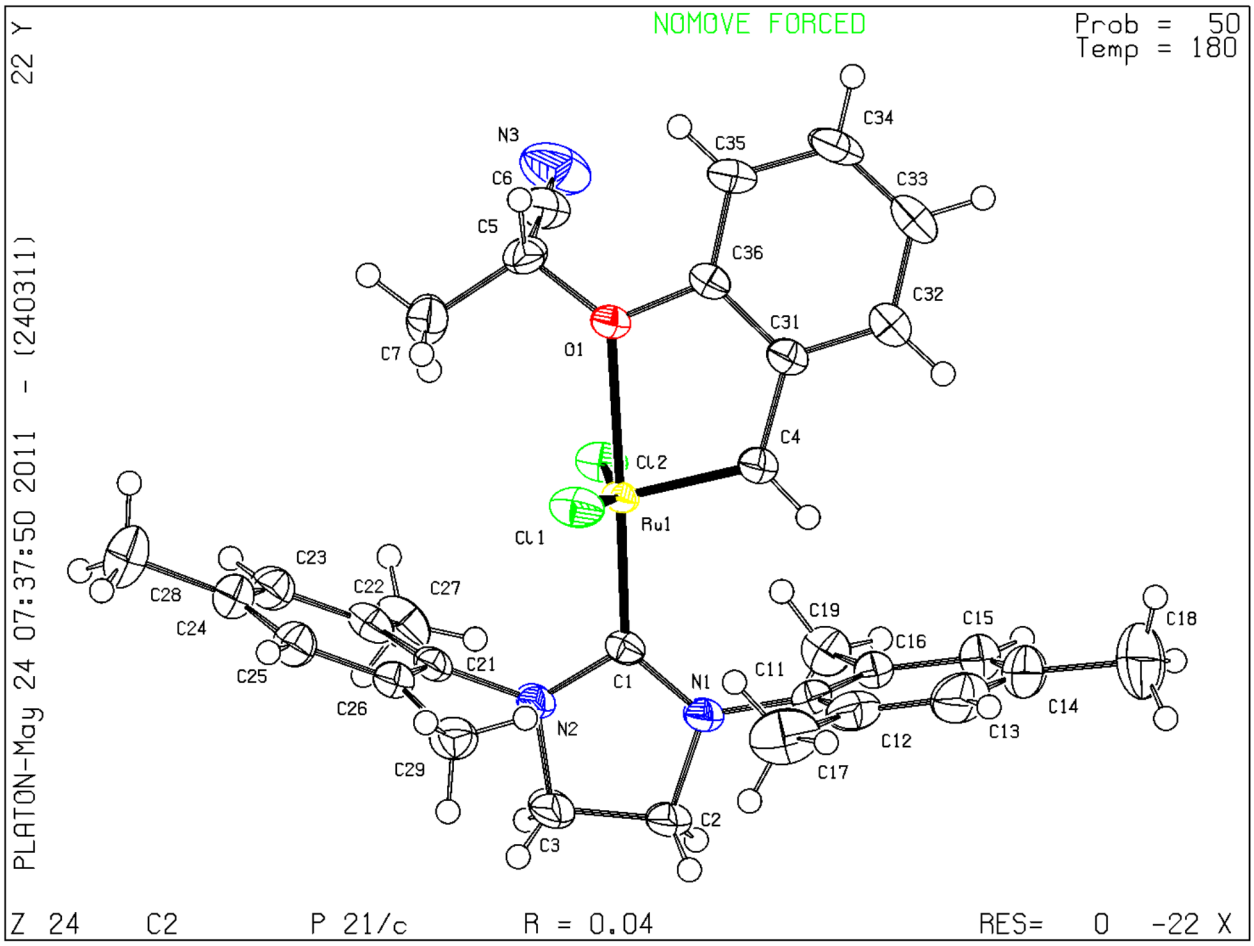
Datablock Kme2 - ellipsoid plot



Datablock M2 - ellipsoid plot



Datablock C2 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry