checkCIF/PLATON report

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

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2

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

Cell:           a=11.3760(3)    b=7.5360(2)         c=11.3800(4)
                alpha=90        beta=101.335(2)     gamma=90
Temperature:    150 K

                Calculated                Reported
Volume          956.57(5)                 956.57(5)
Space group     P 21/c                    P21/c
Hall group      -P 2ybc                   ?
Moiety formula  C11 H15 Co                ?
Sum formula     C11 H15 Co                C11 H15 Co
Mr              206.16                    206.16
Dx,g cm-3       1.431                     1.432
Z               4                         4
Mu (mm-1)       1.734                     1.734
F000            432.0                     432.0
F000'           433.48
h,k,lmax        14,9,14                   14,9,14
Nref            2275                      2211
Tmin,Tmax       0.812,0.870               0.781,0.881
Tmin'           0.771

Correction method= # Reported T Limits: Tmin=0.781 Tmax=0.881
AbsCorr = MULTI-SCAN

Data completeness= 0.972          Theta(max)= 27.880

R(reflections)= 0.0296( 1704)     wR2(reflections)= 0.0564( 2211)

S = 1.038                 Npar= 127
```

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.972 Note

Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 4 Note
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

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

Datablock: 5

Bond precision: C-C = 0.0027 A Wavelength=0.71073

Cell: a=34.6560(1) b=5.8840(3) c=24.1690(4)
alpha=90 beta=131.651(1) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	3682.6(2)	3682.6(2)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C12 H13 Co	?
Sum formula	C12 H13 Co	C24 H26 Co2
Mr	216.15	432.31
Dx,g cm-3	1.559	1.559
Z	16	8
Mu (mm-1)	1.806	1.806
F000	1792.0	1792.0
F000’	1797.95	
h,k,lmax	49,8,34	49,8,34
Nref	5647	5499
Tmin,Tmax	0.754,0.791	0.743,0.806
Tmin’	0.736	

Correction method= # Reported T Limits: Tmin=0.743 Tmax=0.806
AbsCorr = MULTI-SCAN

Data completeness= 0.974 Theta(max)= 30.520

R(reflections)= 0.0287(4368) wR2(reflections)= 0.0707(5499)

S = 1.022 Npar= 289

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full value Low .	0.974 Note
PLAT147_ALERT_1_C	s.u. on Symmetry Constrained Cell Angle(s)	Please Check
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.3 Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	4.4 Ratio

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Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00 Check
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a Note
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	8 Note
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C21A -- C22A ..	9.7 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C22A -- C23A ..	9.7 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C23A -- C24A ..	6.4 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder ..... Percentage =	19 Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	20 Check

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Datablock: 6

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=11.3070(2) b=7.3250(1) c=12.6230(3)
alpha=90 beta=102.883(1) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	1019.17(3)	1019.17(3)
Space group	P 21/a	P21/a
Hall group	-P 2yab	?
Moiety formula	C13 H17 Co	?
Sum formula	C13 H17 Co	C26 H34 Co2
Mr	232.20	464.39
Dx,g cm-3	1.513	1.513
Z	4	2
Mu (mm-1)	1.637	1.637
F000	488.0	488.0
F000’	489.50	
h,k,lmax	16,10,18	16,10,18
Nref	3112	3052
Tmin,Tmax	0.728,0.757	0.735,0.763
Tmin’	0.714	

Correction method= # Reported T Limits: Tmin=0.735 Tmax=0.763
AbsCorr = MULTI-SCAN

Data completeness= 0.981 Theta(max)= 30.500

R(reflections)= 0.0265(2636) wR2(reflections)= 0.0641(3052)

S = 1.067 Npar= 134

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 G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group P21/a P21/c Note
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 1 Note

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT029_2
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.972 Note
RESPONSE: ...
;
_vrf_PLAT029_5
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.974 Note
RESPONSE: ...
;
_vrf_PLAT147_5
;
PROBLEM: s.u. on Symmetry Constrained Cell Angle(s) .....     Please Check
RESPONSE: ...
;
_vrf_PLAT220_5
;
PROBLEM: Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        4.3 Ratio
RESPONSE: ...
;
_vrf_PLAT222_5
;
PROBLEM: Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range        4.4 Ratio
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to 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 purpose of your study may justify the reported deviations and the more serious of these should normally 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.

Publication of your CIF in IUCr journals

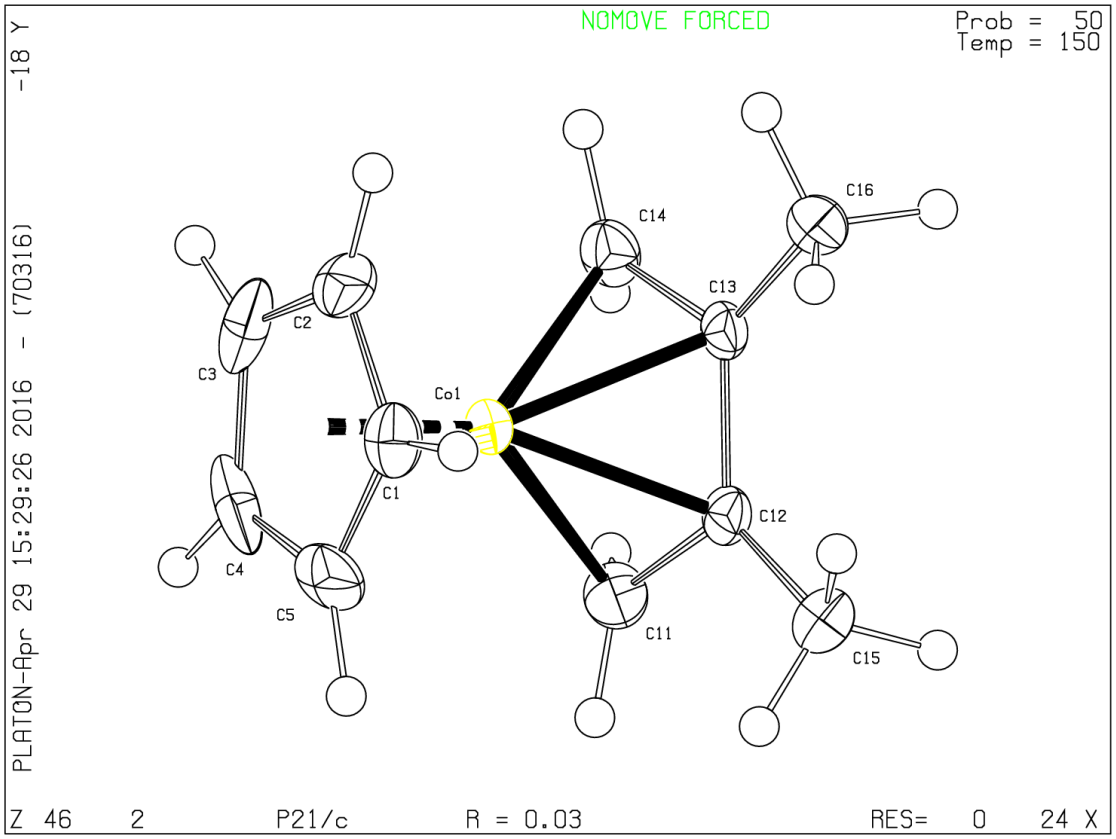
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

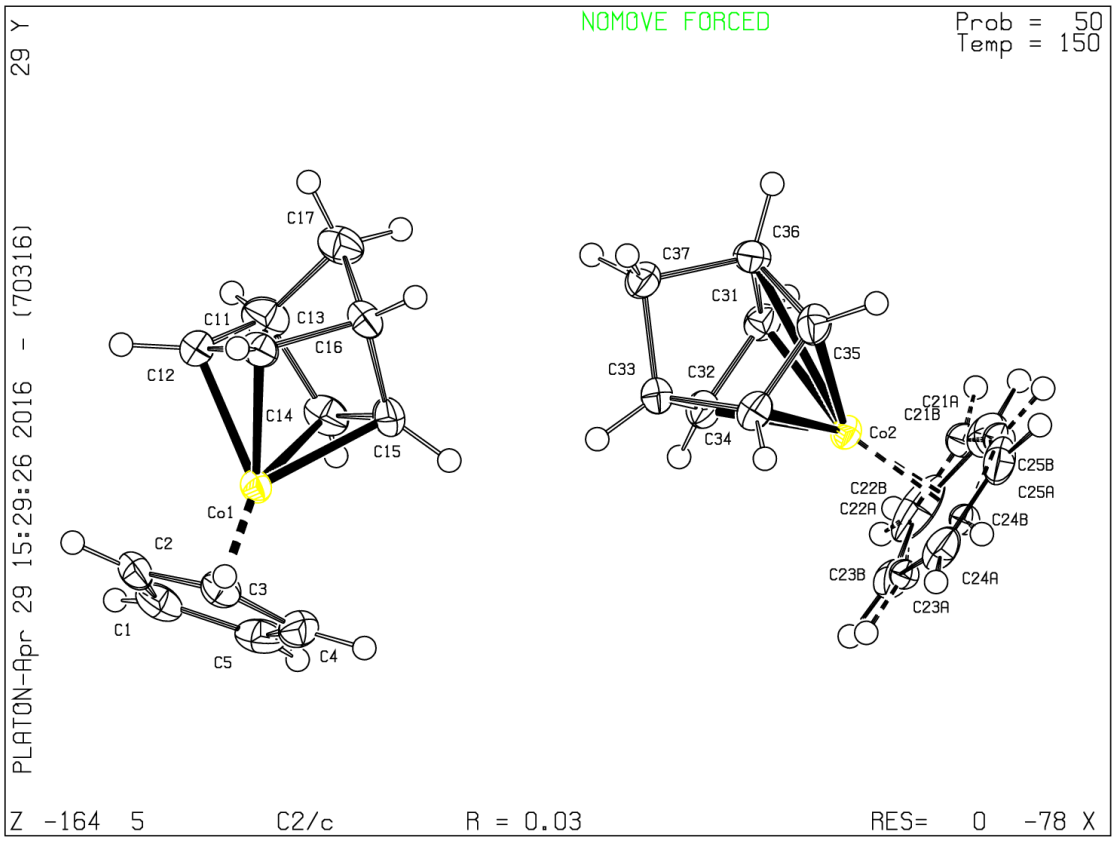
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 30/03/2016; check.def file version of 30/03/2016

Datablock 2 - ellipsoid plot



Datablock 5 - ellipsoid plot



Datablock 6 - ellipsoid plot