

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: 1

Bond precision:	C-C = 0.0045 A	Wavelength=0.71073
Cell:	a=26.118(4)	b=10.9943(18) c=9.1219(15)
	alpha=90	beta=108.954(2) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	2477.3(7)	2477.4(7)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C26 H22 Co N4 O6	?
Sum formula	C26 H22 Co N4 O6	C26 H22 Co N4 O6
Mr	545.41	545.40
Dx, g cm-3	1.462	1.462
Z	4	4
Mu (mm-1)	0.742	0.742
F000	1124.0	1124.0
F000'	1125.87	
h, k, lmax	31, 13, 10	31, 13, 10
Nref	2217	2209
Tmin, Tmax	0.779, 0.825	0.786, 0.830
Tmin'	0.777	

Correction method= # Reported T Limits: Tmin=0.786 Tmax=0.830
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.148

R(reflections)= 0.0373(1634) wR2(reflections)= 0.1030(2209)

S = 1.025 Npar= 174

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Co1 --03 . 5.5 s.u.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II) .	1.84	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	3	Note

- 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
10 **ALERT level G** = General information/check it is not something unexpected
- 3 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
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
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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.

