checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0069 A Wavelength=0.71073

Cell: a=15.7047(16) b=18.2941(17) c=14.4680(14)
alpha=90 beta=91.730(3) gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	4154.8(7)	4154.8(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	?
Moiety formula	2(C37 H26 Co N5 O5), 4(F6 P), C H4 O, H2 O	C37 H26 Co N5 O5, 2(F6 P), 0.5(C H4 O), 0.5(H2 O)
Sum formula	C75 H58 Co2 F24 N10 O12 P4	C37.50 H29 Co1 F12 N5 O6 P2
Mr	1989.05	994.53
Dx,g cm-3	1.590	1.590
Z	2	4
Mu (mm-1)	0.596	0.596
F000	2008.0	2008.0
F000'	2011.58	
h,k,lmax	19,22,17	19,22,17
Nref	7974	7913
Tmin,Tmax	0.892,0.914	0.910,0.910
Tmin'	0.877	

Correction method= # Reported T Limits: Tmin=0.910 Tmax=0.910
AbsCorr = NUMERICAL

Data completeness= 0.992 Theta(max)= 25.762

R(reflections)= 0.0530(5146) wR2(reflections)= 0.1181(5146)

S = 1.000 Npar= 559

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

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.7 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       4.1 Ratio
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00689 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        32 Report
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        28 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         3 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     0.500 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        P1 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        P2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F2         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F3         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F11        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F12        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F13        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F14        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F15        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F16        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F17        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F18        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F19        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F20        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F21        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F22        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F23        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F24        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O6         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C38        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H61        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H381       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H382       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H383       Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O7         Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H71        Constrained at       0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H72        Constrained at       0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        86% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        86% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )       1.50 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O4       .      107.3 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O5       .      103.9 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  F11      ..C35      .       2.81 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F11      ..C14      .       2.94 Ang.
                                                     x,y,z  =      1_555 Check
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data     Please Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
             F6 P
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (III)     .       3.46 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found     Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        42 Note
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         52 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked          ! Info
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...         14 Check
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
57 **ALERT level G** = General information/check it is not something unexpected

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

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 12/09/2022; check.def file version of 09/08/2022

Datablock I - ellipsoid plot

