

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 = 0.0029 A	Wavelength=0.71070
Cell:	a=7.8463(3)	b=16.9377(6) c=15.0047(5)
	alpha=90	beta=103.360(3) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	1940.13(12)	1940.13(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	?
Moiety formula	2(C13 H15 Co N9 O2 S2), C2 H6 O	2(C13 H15 Co N9 O2 S2), C2 H6 O
Sum formula	C28 H36 Co2 N18 O5 S4	C28 H36 Co2 N18 O5 S4
Mr	950.85	950.85
Dx,g cm-3	1.628	1.628
Z	2	2
Mu (mm-1)	1.135	1.135
F000	976.0	976.0
F000'	978.62	
h,k,lmax	10,23,20	10,23,20
Nref	5194	5189
Tmin,Tmax	0.762,0.843	0.980,1.000
Tmin'	0.672	

Correction method= # Reported T Limits: Tmin=0.980 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 29.070

R(reflections)= 0.0351(4358) wR2(reflections)= 0.0891(5189)

S = 1.051 Npar= 275

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

PLAT414_ALERT_2_C	Short Intra D-H..H-X	H6	..H10C	1.98 Ang.
			x,y,z =	1_555 Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N8	--H8B	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N9	--H9B	Please Check

Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found	in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	7 Report
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.		1 Note
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	S1 --C12	7.1 s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	S2 --C13	8.9 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Col --N2	7.6 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of	O3 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C14A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	C14B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H3A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H14A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H14B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H14C Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H14D Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	H14E Constrained at	0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	4.50 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O3 ..C8	2.90 Ang.
		x,1/2-y,-1/2+z =	4_565 Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ...	#	53 Do !
	N1 -CO1 -N2 -C13	137.60 0.60 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ...	#	59 Do !
	CO1 -N2 -C13 -S2	-120.00 8.00 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ...	#	60 Do !
	N2 -CO1 -N1 -C12	55.80 0.90 1.555 1.555 1.555	1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ...	#	104 Do !
	CO1 -N1 -C12 -S1	116.00 7.00 1.555 1.555 1.555	1.555
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group	#	9 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Col	(II)	1.75 Info
PLAT899_ALERT_4_G	SHELXL97	is Deprecated and Succeeded by SHELXL	2018 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 7 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
 18 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

