

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nia006\_150k

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: nia006\_150k

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Bond precision:      C-C = 0.0059 Å      Wavelength=1.54186

Cell:                      a=14.7142 (9)              b=9.8420 (5)              c=25.6400 (17)  
                            alpha=90              beta=94.944 (5)              gamma=90

Temperature:              150 K

	Calculated	Reported
Volume	3699.3 (4)	3699.3 (4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H56 Co N10 O2 S2, 2(C H C13) [+ solvent]	C70 H56 Co N10 O2 S2, 2(C H C13), 1[CHCL3]
Sum formula	C72 H58 Cl6 Co N10 O2 S2 [+ solvent]	C73 H59 Cl9 Co N10 O2 S2
Mr	1431.03	1550.40
Dx, g cm <sup>-3</sup>	1.285	1.392
Z	2	2
Mu (mm <sup>-1</sup> )	4.738	5.755
F000	1474.0	1590.0
F000'	1478.28	
h, k, lmax	18, 12, 31	18, 12, 31
Nref	7390	7229
Tmin, Tmax	0.400, 0.501	0.135, 0.210
Tmin'	0.275	

Correction method= # Reported T Limits: Tmin=0.135 Tmax=0.210

AbsCorr = MULTII-SCAN

Data completeness= 0.978

Theta(max)= 73.075

R(reflections)= 0.0845( 5841)

wR2(reflections)=  
0.2316( 7229)

S = 1.019

Npar= 426

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

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C36	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of	C34	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including C11	0.105	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	22	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		2	Check



### 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: C73 H59 Cl9 Co1 N10 O2 S2  
Atom count from the \_atom\_site data: C72 H58 Cl6 Co1 N10 O2 S2  
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 2  
From the CIF: \_chemical\_formula\_sum C73 H59 Cl9 Co N10 O2 S2  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	146.00	144.00	2.00
H	118.00	116.00	2.00
Cl	18.00	12.00	6.00
Co	2.00	2.00	0.00
N	20.00	20.00	0.00
O	4.00	4.00	0.00
S	4.00	4.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ	Please	Check
PLAT051_ALERT_1_G	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	17.68	%
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	8.00	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	219	A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II) .	1.99	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	135	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	7	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	5	Check

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

4 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  
6 ALERT type 3 Indicator that the structure quality may be low  
5 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

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**PLATON version of 19/02/2022; check.def file version of 19/02/2022**

