

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) nia003\_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: nia003\_150k

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Bond precision:	C-C = 0.0078 A	Wavelength=1.54186	
Cell:	a=13.3183 (3)	b=12.5045 (2)	c=15.2418 (4)
	alpha=90	beta=96.533 (2)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	2521.87 (10)	2521.87 (10)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C52 H48 Co N10 S2, 0.8 (C H C13)	C52 H50 Co N10 S2, 0.8 (C H C13)	
Sum formula	C52.80 H48.80 Cl2.40 Co N10 S2	C52.80 H48.80 Cl2.40 Co N10 S2	
Mr	1031.55	1031.55	
Dx, g cm <sup>-3</sup>	1.359	1.358	
Z	2	2	
Mu (mm <sup>-1</sup> )	4.982	4.982	
F000	1070.8	1071.0	
F000'	1071.56		
h, k, lmax	16, 15, 18	16, 15, 18	
Nref	5021	4963	
Tmin, Tmax	0.384, 0.451	0.032, 0.063	
Tmin'	0.291		

Correction method= # Reported T Limits: Tmin=0.032 Tmax=0.063

AbsCorr = MULTI-SCAN

Data completeness= 0.988

Theta (max)= 72.668

R(reflections)= 0.1030( 4678)

wR2(reflections)=  
0.2400( 4963)

S = 0.941

Npar= 377

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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.

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### Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00779 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.737 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	10 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	13 Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	18.60 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.06Ang From Cl3	1.95 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.86Ang From Cl2	1.83 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.36Ang From Cl2	-1.76 eA-3

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### Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C52.8 H48.8 Cl2.4 Co1 N10 S2  
Atom count from \_chemical\_formula\_moiety:C52.8 H50.8 Cl2.4 Co1 N10 S2

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	15.00 Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	6 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	3 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of N4 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N5 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C26 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C27 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C30 Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C31 Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C32 Constrained at	0.45 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3 Constrained at	0.55 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A Constrained at	0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H27C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H30	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H31	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H32	Constrained at	0.45	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C29	Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H29	Constrained at	0.4	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )		18%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT410_ALERT_2_G	Short Intra H...H Contact H18 ..H24A .		2.00	Ang.
	x,y,z =	1_555	Check	
PLAT410_ALERT_2_G	Short Intra H...H Contact H20 ..H22A .		2.07	Ang.
	x,y,z =	1_555	Check	
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H23B ..H25A .		1.97	Ang.
	x,y,z =	1_555	Check	
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		5	Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters		1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		73	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		49	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		4.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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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  
 10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 59 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 8 ALERT type 3 Indicator that the structure quality may be low  
 46 ALERT type 4 Improvement, methodology, query or suggestion  
 1 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.

