

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) datam

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: datam

Bond precision: C-C = 0.0125 Å Wavelength=1.54184

Cell: a=5.7751(6) b=46.275(3) c=7.7780(8)
 alpha=90 beta=90.655(10) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	2078.5(3)	2078.5(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H24 N2 S	?
Sum formula	C26 H24 N2 S	C26 H24 Cl0 N2 O0 S
Mr	396.53	396.53
Dx, g cm ⁻³	1.267	1.267
Z	4	4
Mu (mm ⁻¹)	1.476	1.476
F000	840.0	840.0
F000'	843.34	
h, k, lmax	7, 56, 9	6, 55, 9
Nref	3889	2774
Tmin, Tmax	0.767, 0.863	
Tmin'	0.767	

Correction method= Not given

Data completeness= 0.713 Theta(max)= 69.646

R(reflections)= 0.1178(1696)

wR2(reflections)=
0.3474(2774)

S = 1.119

Npar= 263

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 A**

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.729 Why?

Author Response: Poorly diffracting crystal. Used only to authenticate atom-connectivit

 **Alert level B**

PLAT031_ALERT_4_B Refined Extinction Parameter Within Range of ... 2.333 Sigma
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01254 Ang.
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 1017 Report

 **Alert level C**

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.13 Do !
PLAT082_ALERT_2_C High R1 Value 0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.35 Report
PLAT213_ALERT_2_C Atom C4 has ADP max/min Ratio 3.1 oblate
PLAT213_ALERT_2_C Atom C9 has ADP max/min Ratio 3.5 oblate
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.1 Note
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 27.541 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.881 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.023 Check

 **Alert level G**

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 4

From the CIF: _chemical_formula_sum C26 H24 Cl0 N2 O0 S

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	104.00	104.00	0.00
H	96.00	96.00	0.00
Cl	4.00	0.00	4.00
N	8.00	8.00	0.00
O	4.00	0.00	4.00
S	4.00	4.00	0.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 29 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 17.77 Why ?
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 407 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	94	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	1.3	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0	Info

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 3 **ALERT level B** = A potentially serious problem, consider carefully
 - 11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 13 **ALERT level G** = General information/check it is not something unexpected
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- 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
 - 10 ALERT type 3 Indicator that the structure quality may be low
 - 7 ALERT type 4 Improvement, methodology, query or suggestion
 - 0 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.

PLATON version of 10/05/2023; check.def file version of 10/05/2023

Datablock datam - ellipsoid plot

