

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) am_sn_11

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: am_sn_11

Bond precision:	C-C = 0.0021 A	Wavelength=0.71073
Cell:	a=8.7296(6)	b=11.1447(6) c=12.3411(6)
	alpha=70.914(2)	beta=86.955(2) gamma=74.653(2)
Temperature:	100 K	
	Calculated	Reported
Volume	1093.45(11)	1093.45(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H23 N3 [+ solvent]	C27 H23 N3, 0.5[C2H6O]
Sum formula	C27 H23 N3 [+ solvent]	C28 H26 N3 O0.5
Mr	389.48	412.54
Dx,g cm-3	1.183	1.253
Z	2	2
Mu (mm-1)	0.070	0.076
F000	412.0	438.2
F000'	412.14	
h,k,lmax	10,13,15	10,13,15
Nref	4304	4234
Tmin,Tmax	0.985,0.992	0.695,0.745
Tmin'	0.972	

Correction method= # Reported T Limits: Tmin=0.695 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 26.010

R(reflections)= 0.0442(3857) wR2(reflections)= 0.1088(4234)

S = 1.066 Npar= 271

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.137 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 50 Report

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: C28 H26 N3 O0.5
Atom count from the _atom_site data: C27 H23 N3
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 C28 H26 N3 O0.5
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	56.00	54.00	2.00
H	52.00	46.00	6.00
N	6.00	6.00	0.00
O	1.00	0.00	1.00

PLAT041_ALERT_1_G Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT073_ALERT_1_G H-atoms ref, but _hydrogen_treatment Reported as		constr Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal..(Note)		0.002 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure		101 A**3
PLAT650_ALERT_4_G SWAT Instruction Used to Model Solvent Disorder		! Report
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data		Please Note
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters		2 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		20 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ...		2 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		8 Info

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

