

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cm_mnt_0m

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: cm_mnt_0m

Bond precision: C-C = 0.0086 Å Wavelength=0.71073

Cell: a=13.7182(5) b=18.3443(7) c=17.4906(6)
 alpha=90 beta=92.414(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4397.6(3)	4397.6(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C32 Cm2 N16 S16, 12(C2 N), 10(Na)	C28 Cm N14 Na5 S8
Sum formula	C56 Cm2 N28 Na10 S16	C28 Cm N14 Na5 S8
Mr	2295.82	1147.85
Dx, g cm ⁻³	1.734	1.734
Z	2	4
Mu (mm ⁻¹)	2.322	2.322
F000	2180.0	2180.0
F000'	2155.55	
h,k,lmax	21,28,26	21,28,26
Nref	16878	16847
Tmin,Tmax	0.677,0.846	0.614,0.747
Tmin'	0.664	

Correction method= # Reported T Limits: Tmin=0.614 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 33.233

R(reflections)= 0.0390(13676)

wR2(reflections)=
0.0878(16847)

S = 1.069

Npar= 505

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 B

PLAT976_ALERT_2_B Check Calcd Resid. Dens. 1.04Ang From C28 . -1.80 eA-3

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C32 Cm2 N16 S16, 12(C2 N), 10(Na)
Rep.: C28 Cm N14 Na5 S8

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C19 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C21 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C25 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C27 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N10 0.128 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N13 0.128 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N14 0.158 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00861 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.341 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
0 2 0, 1 0 1,

PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
-1 2 2,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.61Ang From Cm1 1.74 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.41Ang From N10 1.61 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.70Ang From Cm1 1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.04Ang From C28 -1.80 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Cm1 1.23 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.95Ang From N10 . 1.11 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.93Ang From C28 . 1.05 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.89Ang From C28 . 0.73 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 18.10 Why ?
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
0 1 1,

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 25 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
0 2 0,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.273 Note
Predicted wR2: Based on SigI**2 3.86 or SHELX Weight 8.21
PLAT983_ALERT_1_G The Cm-f"= 4.8980 Deviates from IT-Value = 4.6980 Check

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT976_cm_mnt_0m
;
PROBLEM: Check Calcd Resid. Dens. 1.04Ang From C28 . -1.80 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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 15/07/2024; check.def file version of 15/07/2024

Datablock cm_mnt_0m - ellipsoid plot

