

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SKM265_0m_a

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: SKM265_0m_a

Bond precision: C-C = 0.0017 Å Wavelength=0.71073

Cell: a=10.0768 (4) b=10.4188 (4) c=11.3759 (5)
 alpha=78.519 (1) beta=82.891 (1) gamma=65.707 (1)
Temperature: 120 K

	Calculated	Reported
Volume	1065.63 (8)	1065.63 (8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H15 N2 O2 S, C5 H12 N	C18 H15 N2 O2 S, C5 H12 N
Sum formula	C23 H27 N3 O2 S	C23 H27 N3 O2 S
Mr	409.54	409.53
Dx, g cm ⁻³	1.276	1.276
Z	2	2
Mu (mm ⁻¹)	0.176	0.176
F000	436.0	436.0
F000'	436.41	
h, k, lmax	13, 14, 15	13, 14, 15
Nref	5777	5673
Tmin, Tmax	0.948, 0.971	0.820, 0.900
Tmin'	0.948	

Correction method= # Reported T Limits: Tmin=0.820 Tmax=0.900
AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 29.187

R(reflections)= 0.0390 (4716)	wR2(reflections)=
S = 1.114	0.1154 (5673)
Npar= 370	

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.19	Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for S1 --C1 .	5.4	s.u.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4	Report



Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C2 --C6 .	6.4	s.u.
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	100	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	16	Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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_PLAT094_SKM265_0m_a
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....      2.19 Report
RESPONSE: ...
;
_vrf_PLAT230_SKM265_0m_a
;
PROBLEM: Hirshfeld Test Diff for      S1      --C1      .      5.4 s.u.
RESPONSE: ...
;
_vrf_PLAT911_SKM265_0m_a
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      4 Report
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.

