

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dm-skp-3-143_cu

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: dm-skp-3-143_cu

Bond precision:	C-C = 0.0079 Å	Wavelength=1.54184
Cell:	a=13.2962 (5)	b=15.7733 (7) c=27.5418 (11)
	alpha=90	beta=98.192 (4) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	5717.3 (4)	5717.3 (4)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C35 H32 N2 O3	0.32 (C35 H32 N2 O3)
Sum formula	C35 H32 N2 O3	C11.20 H10.24 N0.64 O0.96
Mr	528.63	169.16
Dx, g cm ⁻³	1.228	1.228
Z	8	25
Mu (mm ⁻¹)	0.619	0.619
F000	2240.0	2240.0
F000'	2246.41	
h, k, lmax	16, 19, 34	16, 19, 33
Nref	11426	11142
Tmin, Tmax	0.971, 0.988	0.241, 1.000
Tmin'	0.923	

Correction method= # Reported T Limits: Tmin=0.241 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.975 Theta (max)= 72.965

R(reflections)= 0.1050 (4698)	wR2(reflections)=
S = 0.988	0.3908 (11142)
Npar= 729	

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

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.39 Report



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.140
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.140 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 42% Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N00E Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00791 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 21.220 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.993 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 9 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 21.24 Check



Alert level G

PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.3200 Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 141 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 274 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected
- 2 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
11 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
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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.

