

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dm_skp_3_226_autored

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_226_autored

Bond precision:	C-C = 0.0028 A	Wavelength=0.71073
Cell:	a=13.5870 (8)	b=7.5797 (4) c=17.5157 (11)
	alpha=90	beta=105.850 (7) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	1735.28 (19)	1735.28 (18)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C22 H19 N O3	0.571 (C22 H19 N O3)
Sum formula	C22 H19 N O3	C12.57 H10.86 N0.57 O1.71
Mr	345.38	197.36
Dx, g cm ⁻³	1.322	1.322
Z	4	7
Mu (mm ⁻¹)	0.088	0.088
F000	728.0	728.0
F000'	728.34	
h, k, lmax	21, 11, 27	21, 11, 27
Nref	6980	6540
Tmin, Tmax	0.992, 0.995	0.574, 1.000
Tmin'	0.992	

Correction method= # Reported T Limits: Tmin=0.574 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.937 Theta (max)= 33.829

R(reflections)= 0.0790 (2930)	wR2(reflections)=
S = 1.012	0.1797 (6540)
Npar= 238	

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

RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.219

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.219 Report



Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 45% Check

PLAT230_ALERT_2_C Hirshfeld Test Diff for N004 --C00H 5.5 s.u.

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 24.956 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 7.792 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.887 Check



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the

_chemical_formula_sum and _chemical_formula_moiety. This is

usually due to the moiety formula being in the wrong format.

Atom count from _chemical_formula_sum: C12.57 H10.86 N0.57 O1.71

Atom count from _chemical_formula_moiety: C12.562 H10.849 N0.571 O1.713

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: _cell_formula_units_Z 7

From the CIF: _chemical_formula_sum C12.57 H10.86 N0.57 O1.71

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
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C	87.99	88.00	-0.01
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H	76.02	76.00	0.02
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N	3.99	4.00	-0.01
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O	11.97	12.00	-0.03
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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 ... 0.5714 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 45 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 440 Note

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully

5 **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

5 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

6 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

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.

