

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dm-skp2-148-2\_mo

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-skp2-148-2\_mo

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Bond precision:	C-C = 0.0052 A	Wavelength=0.71073
Cell:	a=17.8628 (16)	b=7.3882 (5)      c=16.1222 (14)
	alpha=90	beta=104.518 (9)      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2059.8 (3)	2059.8 (3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C25 H27 N O2	0.444 (C25 H27 N O2)
Sum formula	C25 H27 N O2	C11.11 H12 N0.44 O0.89
Mr	373.48	165.99
Dx, g cm <sup>-3</sup>	1.204	1.204
Z	4	9
Mu (mm <sup>-1</sup> )	0.076	0.076
F000	800.0	800.0
F000'	800.33	
h, k, lmax	21, 8, 19	21, 8, 19
Nref	3623	3622
Tmin, Tmax	0.994, 0.997	0.510, 1.000
Tmin'	0.994	

Correction method= # Reported T Limits: Tmin=0.510 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.000      Theta(max)= 25.000

R(reflections)= 0.0756 ( 2156)	wR2(reflections)= 0.2949 ( 3622)
S = 0.952	Npar= 258

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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.

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### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12

Rint given 0.137

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12 .....	0.137	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.29	Report
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0052	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	12.352	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.216	Check
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	3	Check
PLAT939_ALERT_3_C	Large Value of Not (SHELXL) Weight Optimized S .	25.31	Check

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### 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: C11.11 H12 N0.44 O0.89

Atom count from \_chemical\_formula\_moiety:C11.1 H11.988 N0.444 O0.888

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 9

From the CIF: \_chemical\_formula\_sum C11.11 H12 N0.44 O0.89

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	99.99	100.00	-0.01
H	108.00	108.00	0.00
N	3.96	4.00	-0.04
O	8.01	8.00	0.01

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 ...	0.4444	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 .....	55	Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	31%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

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

8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

11 **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

10 ALERT type 3 Indicator that the structure quality may be low

1 ALERT type 4 Improvement, methodology, query or suggestion

1 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.

