

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dm_skp_3_145

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_145

Bond precision:	C-C = 0.0030 A	Wavelength=0.71073
Cell:	a=7.1271 (4)	b=24.7374 (15) c=13.8207 (9)
	alpha=90	beta=101.066 (6) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2391.4 (3)	2391.4 (3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C29 H27 F N2 O3	0.4 (C29 H27 F N2 O3)
Sum formula	C29 H27 F N2 O3	C11.60 H10.80 F0.40 N0.80 O1.20
Mr	470.53	188.21
Dx, g cm ⁻³	1.307	1.307
Z	4	10
Mu (mm ⁻¹)	0.090	0.090
F000	992.0	992.0
F000'	992.48	
h, k, lmax	10, 37, 21	10, 37, 21
Nref	8976	7361
Tmin, Tmax	0.994, 0.996	0.285, 1.000
Tmin'	0.992	

Correction method= # Reported T Limits: Tmin=0.285 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.820 Theta(max)= 32.937

R(reflections)= 0.0741 (3503)	wR2(reflections)= 0.1790 (7361)
S = 1.030	Npar= 320

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.152

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.152	Report
PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	48%	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	12.481	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.058	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	2	Report



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 ...	0.4000	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	61	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1612	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **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
- 2 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
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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.

