

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dmsolgjx

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: dmsolgjx

Bond precision:	C-C = 0.0036 A	Wavelength=1.54178
Cell:	a=9.2108 (6)	b=15.0939 (11) c=18.0815 (12)
	alpha=90	beta=90 gamma=90
Temperature:	170 K	
	Calculated	Reported
Volume	2513.8 (3)	2513.8 (3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C23 H32 F3 N5 O4	C23 H32 F3 N5 O4
Sum formula	C23 H32 F3 N5 O4	C23 H32 F3 N5 O4
Mr	499.54	499.53
Dx, g cm ⁻³	1.320	1.320
Z	4	4
Mu (mm ⁻¹)	0.901	0.901
F000	1056.0	1056.0
F000'	1059.74	
h, k, lmax	11, 18, 22	11, 18, 22
Nref	5180 [2933]	5115
Tmin, Tmax	0.823, 0.947	0.598, 0.754
Tmin'	0.820	

Correction method= # Reported T Limits: Tmin=0.598 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 1.74/0.99 Theta(max)= 74.878

R(reflections)= 0.0433 (4971)	wR2(reflections)=
S = 1.050	0.1147 (5115)
Npar= 321	

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

PLAT230_ALERT_2_C Hirshfeld Test Diff for F3 --C23 . 6.5 s.u.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT791_ALERT_4_G Model has Chirality at C4 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C6 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C9 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C10 (Sohnke SpGr) R Verify
PLAT791_ALERT_4_G Model has Chirality at C11 (Sohnke SpGr) S Verify
PLAT791_ALERT_4_G Model has Chirality at C17 (Sohnke SpGr) S Verify
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 20 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
8 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.

