



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CEC0526

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: CEC0526

Bond precision:	C-C = 0.0007 Å	Wavelength=0.71073	
Cell:	a=7.0917 (15) alpha=90	b=20.475 (4) beta=102.129 (7)	c=9.212 (2) gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	1307.8 (5)	1307.7 (5)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C14 H19 F2 N O	C14 H19 F2 N O	
Sum formula	C14 H19 F2 N O	C14 H19 F2 N O	
Mr	255.30	255.30	
Dx, g cm-3	1.297	1.297	
Z	4	4	
Mu (mm-1)	0.100	0.100	
F000	544.0	544.0	
F000'	544.31		
h, k, lmax	14, 41, 18	14, 40, 18	
Nref	11027	10962	
Tmin, Tmax	0.986, 0.991	0.940, 0.990	
Tmin'	0.976		

Correction method= # Reported T Limits: Tmin=0.940 Tmax=0.990
AbsCorr = NUMERICAL

Data completeness= 0.994

Theta(max)= 45.420

R(reflections)= 0.0395(8763)

wR2(reflections)=
0.1248(10962)

S = 1.037

Npar= 172

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.08	Report
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N18 --H18A .		Please Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4	Report
	3 6 3, 3 9 3, 1 14 3, 3 0 6,		



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	1	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0100	Report
PLAT793_ALERT_4_G	Model has Chirality at C8 (Centro SpGr)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	61	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	2	Note
	3 9 3, 3 6 3,		
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	91.0	Degree
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.731	Note
	Predicted wR2: Based on SigI**2 2.64 or SHELX Weight 12.04		Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	12	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	6	Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **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
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
3 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 23/04/2026; check.def file version of 30/03/2026

duplicate check

No duplication found

Datablock CEC0526 - ellipsoid plot

