



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4c

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: 4c

Bond precision:	C-C = 0.0033 Å	Wavelength=1.54184
Cell:	a=15.8110 (6)	b=6.50949 (18) c=18.9382 (7)
	alpha=90	beta=114.495 (4) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	1773.72 (12)	1773.71 (12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C19 H9 F9 N2 O2	C19 H9 F9 N2 O2
Sum formula	C19 H9 F9 N2 O2	C19 H9 F9 N2 O2
Mr	468.28	468.28
Dx, g cm ⁻³	1.754	1.754
Z	4	4
Mu (mm ⁻¹)	1.612	1.612
F000	936.0	936.0
F000'	940.50	
h, k, lmax	19, 7, 22	19, 7, 22
Nref	3241	3212
Tmin, Tmax	0.737, 0.882	0.799, 1.000
Tmin'	0.372	

Correction method= # Reported T Limits: Tmin=0.799 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 67.976

R(reflections)= 0.0559(2703)

wR2(reflections)=
0.1577(3212)

S = 1.056

Npar= 289

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

PLAT790_ALERT_4_C Centre of Gravity not Within Unit-Cell: Resd. # 1 Note
C19 H9 F9 N2 O2
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 17 Report
-18 1 3, -14 5 3, -16 3 4, -12 6 4, -8 7 4, -5 0 4,
-12 4 5, 4 7 6, -2 1 7, 3 7 7, 2 0 8, -4 7 10,
-3 7 10, -14 5 11, -15 4 12, -14 4 16, -10 0 22,



Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
H1 H2
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT242_ALERT_2_G Low MainResAtom Ueq as Compared to Neighbours C1 Check
PLAT242_ALERT_2_G Low MainResAtom Ueq as Compared to Neighbours C17 Check
PLAT242_ALERT_2_G Low MainResAtom Ueq as Compared to Neighbours C18 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O2 ..C2 2.96 Ang.
1-x,-1/2+y,1/2-z = 2_645 Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 74% Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.9 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.627 Note
Predicted wR2: Based on SigI**2 4.35 or SHELX Weight 14.93
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info
PLAT994_ALERT_1_G SHELXL .ins Contains no or MERG 0 Instruction .. ! Note

- 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
12 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 15/01/2026; check.def file version of 02/01/2026

Datablock 4c - ellipsoid plot

