

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bmk1777e

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: bmk1777e

Bond precision: C-C = 0.0079 A Wavelength=0.71073

Cell: a=7.7607(3) b=18.2950(11) c=19.5252(14)
 alpha=115.910(6) beta=96.971(4) gamma=92.567(4)

Temperature: 293 K

	Calculated	Reported
Volume	2460.2(3)	2460.2(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H19 Br F2 N6 S	?
Sum formula	C27 H19 Br F2 N6 S	C54 H38 Br2 F4 N12 S2
Mr	577.44	1154.90
Dx,g cm-3	1.559	1.559
Z	4	2
Mu (mm-1)	1.801	1.801
F000	1168.0	1168.0
F000'	1167.77	
h,k,lmax	10,25,27	10,25,25
Nref	14079	11617
Tmin,Tmax	0.734,0.809	0.993,0.997
Tmin'	0.322	

Correction method= # Reported T Limits: Tmin=0.993 Tmax=0.997
AbsCorr = GAUSSIAN

Data completeness= 0.825 Theta(max)= 29.782

R(reflections)= 0.0669(5906) wR2(reflections)= 0.2137(11617)

S = 1.032 Npar= 669

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**

PLAT334_ALERT_2_C	Small Aver. Benzene C-C Dist C22	-C27	1.37 Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00787 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H17	..N10	2.65 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H17	..N11	2.66 Ang.
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...		-2.154 Report

● **Alert level G**

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		2.00 Check
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size ..		0.62 mm
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	(K)	293 Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Br2	..F1	3.01 Ang.
		1-x,1-y,2-z =	2_667 Check
PLAT793_ALERT_4_G	Model has Chirality at C10	(Centro SPGR)	R Verify
PLAT793_ALERT_4_G	Model has Chirality at C37	(Centro SPGR)	S Verify
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		2371 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.0 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ		2 Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ		2 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0 Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		3 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected

5 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
4 ALERT type 3 Indicator that the structure quality may be low
6 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. 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.

PLATON version of 22/03/2021; check.def file version of 19/03/2021

