

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lumateperonetosylate

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: lumateperonetosylate

Bond precision:	C-C = 0.0103 Å	Wavelength=1.34139	
Cell:	a=15.626(3)	b=6.0806(10)	c=31.415(5)
	alpha=90	beta=96.609(7)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	2965.1(9)	2965.1(8)	
Space group	C 2	C 1 2 1	
Hall group	C 2y	C 2y	
Moiety formula	C24 H29 F N3 O, C7 H7 O3 S	C24 H29 F N3 O, C7 H7 O3 S	
Sum formula	C31 H36 F N3 O4 S	C31 H36 F N3 O4 S	
Mr	565.69	565.69	
Dx, g cm ⁻³	1.267	1.267	
Z	4	4	
Mu (mm ⁻¹)	0.878	0.878	
F000	1200.0	1200.0	
F000'	1203.83		
h, k, lmax	18, 7, 37	18, 7, 37	
Nref	5438 [2998]	5411	
Tmin, Tmax	0.934, 0.963	0.552, 0.752	
Tmin'	0.850		

Correction method= # Reported T Limits: Tmin=0.552 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 1.80/1.00 Theta(max)= 53.900

R(reflections)= 0.0807(2903)	wR2(reflections)= 0.2403(5411)
S = 0.987	Npar= 340

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 B**

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01031 Ang.

Author Response: The low bond precision is caused by thermal vibration because of collecting temperature (room temperature).

 **Alert level C**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.141

Author Response: The high Rint value is caused by the poor crystal data quality and collecting temperature.

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 0.141 Report

Author Response: The high Rint value is caused by the poor crystal data quality and collecting temperature.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including F1 0.114 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S1 0.111 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.933 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report

 **Alert level G**

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 17 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0050 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0020 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0010 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0020 Report

PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar	0.0020	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	106	Note
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).	1	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.	0	Info

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
16 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT241_lumateperonetosylate
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of          C2 Check
RESPONSE: ...
;
_vrf_PLAT242_lumateperonetosylate
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of          C1 Check
RESPONSE: ...
;
_vrf_PLAT260_lumateperonetosylate
;
PROBLEM: Large Average Ueq of Residue Including          F1          0.114 Check
RESPONSE: ...
;
_vrf_PLAT906_lumateperonetosylate
;
PROBLEM: Large K Value in the Analysis of Variance .....          3.933 Check
RESPONSE: ...
;
_vrf_PLAT911_lumateperonetosylate
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=          0.600          5 Report
RESPONSE: ...
;
# end Validation Reply Form
```

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.

