checkCIF/PLATON report

Structure factors have been supplied for datablock(s) naj3_autoshape

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: naj3_autoshape

Bond precision: C-C = 0.0020 A   Wavelength=1.54184

Cell: a=7.9650(3)   b=11.6008(4)   c=11.7281(4)
                 alpha=71.646(3)   beta=83.951(3)   gamma=73.737(3)
Temperature: 100 K

	Calculated	Reported
Volume	987.22(6)	987.23(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C38 H34 F12 N8 O8	C38 H34 F12 N8 O8
Sum formula	C38 H34 F12 N8 O8	C38 H34 F12 N8 O8
Mr	958.73	958.73
Dx,g cm-3	1.613	1.613
Z	1	1
Mu (mm-1)	1.340	1.340
F000	490.0	490.0
F000'	492.12	
h,k,lmax	9,14,14	9,14,14
Nref	4020	3960
Tmin,Tmax	0.923,0.935	0.876,1.000
Tmin'	0.706	

Correction method= # Reported T Limits: Tmin=0.876 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.985   Theta(max)= 74.466

R(reflections)= 0.0359(3519)   wR2(reflections)= 0.0992(3960)

S = 0.969   Npar= 298

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.

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Alert level C
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   5 Report

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Alert level G
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   1 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.003 Degree
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C3A Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT898_ALERT_4_G Second Reported H-M Symbol in CIF Ignored ......   ! Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   55 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   3.0 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   9 Info

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   0 **ALERT level A** = Most likely a serious problem – resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   1 **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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   2 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.

PLATON version of 19/02/2022; check.def file version of 19/02/2022