checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rf1690

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: rf1690

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Bond precision:  C-C = 0.0049 A          Wavelength=0.71073

Cell:            a=20.1848(6)     b=11.9034(3)     c=19.6102(6)
                 alpha=90         beta=90          gamma=90
Temperature:     100 K

                Calculated                Reported
Volume          4711.7(2)                 4711.7(2)
Space group     P c a 21                  P c a 21
Hall group      P 2c -2ac                 P 2c -2ac
Moiety formula  C54 H36 F9 N2 O6 Pr       C54 H36 F9 N2 O6 Pr
Sum formula     C54 H36 F9 N2 O6 Pr       C54 H36 F9 N2 O6 Pr
Mr              1120.76                   1120.76
Dx,g cm-3       1.580                     1.580
Z               4                         4
Mu (mm-1)       1.124                     1.124
F000            2248.0                    2248.0
F000'           2248.46
h,k,lmax        28,16,27                  28,16,27
Nref            13733[ 7056]              13727
Tmin,Tmax       0.784,0.864               0.733,0.900
Tmin'           0.755

Correction method= # Reported T Limits: Tmin=0.733 Tmax=0.900
AbsCorr = MULTI-SCAN

Data completeness= 1.95/1.00      Theta(max)= 29.995

R(reflections)= 0.0266( 12338)    wR2(reflections)= 0.0534( 13727)

S = 1.029                 Npar= 651
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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

PLAT213_ALERT_2_C Atom F7 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom F9 has ADP max/min Ratio ..... 3.4 prolat

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C29 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5 ..F9 2.74 Ang.
1-x,1-y,1/2+z = 2_665 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pr1 (III) . 3.64 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 7 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). 4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note
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. 7 Info

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
8 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 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 08/07/2020; check.def file version of 17/06/2020

Datablock rf1690 - ellipsoid plot