checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rf1758

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: rf1758

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Bond precision:   C-C = 0.0044 A            Wavelength=0.71073

Cell:           a=8.9307(4)     b=28.9448(12)        c=16.2421(7)
                alpha=90        beta=105.674(2)      gamma=90
Temperature:    100 K

                Calculated                  Reported
Volume          4042.4(3)                   4042.4(3)
Space group     P 21/c                      P 21/c
Hall group      -P 2ybc                     -P 2ybc
Moiety formula  C44 H32 F9 O8 Pr            C44 H32 F9 O8 Pr
Sum formula     C44 H32 F9 O8 Pr            C44 H32 F9 O8 Pr
Mr              1000.61                     1000.60
Dx,g cm-3       1.644                       1.644
Z               4                           4
Mu (mm-1)       1.301                       1.301
F000            2000.0                      2000.0
F000'           2000.44
h,k,lmax        12,40,22                    12,40,22
Nref            11893                       11826
Tmin,Tmax       0.804,0.890                 0.776,0.933
Tmin'           0.791

Correction method= # Reported T Limits: Tmin=0.776 Tmax=0.933
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 30.110

R(reflections)= 0.0437( 10371)    wR2(reflections)= 0.0853( 11826)

S = 1.243                  Npar= 567
```

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
PLAT930_ALERT_2_B FCF-based   Twin Law (0 0 1)[1 0 2] Est.d BASF   0.02 Check

Alert level C
PLAT354_ALERT_3_C Short O-H (X0.82,N0.98A) O8   - H2O   .   0.70 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   5.797 Check

Alert level G
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   10.36 Why ?
PLAT794_ALERT_5_G Tentative Bond Valency for Pr1   (III)   .   3.49 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..   ! Info
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   64 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law   [1 0 2] Est.d BASF   0.02 Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

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

   1 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
   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. 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
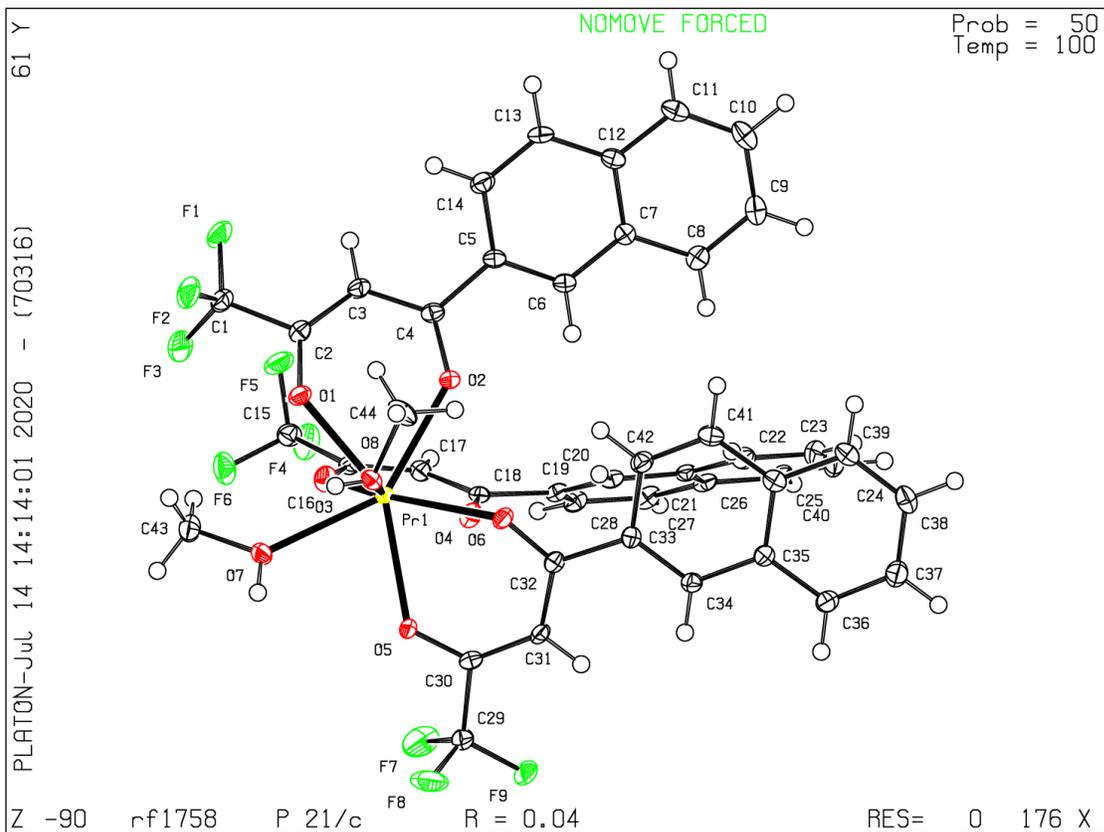
Alert level B
PLAT930_ALERT_2_B FCF-based Twin Law (0 0 1)[1 0 2] Est.d BASF 0.02 Check

RESPONSE: Attempt of twin refinement did not improve structural model.